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COMPUTATIONS OF SOOT AND NO_x EMISSIONS FROM GAS TURBINE COMBUSTORS

FINAL REPORT

by

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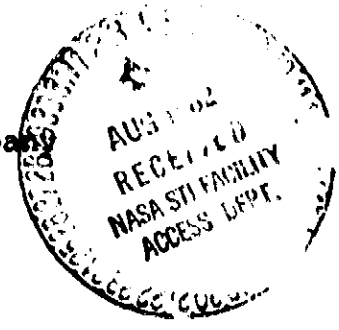

Prepared for

National Aeronautics and Space Administration
NASA-Lewis Research Center
Cleveland, Ohio 44135

Contract No. NAS3-22542

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FOREWORD

This document is the final report for work performed by the Garrett Turbine Engine Company under Contract NAS3-22542. This program, under the sponsorship of the National Aeronautics and Space Administration (NASA) Lewis Research Center accomplished the technical effort involved in the computations of emissions using a 3-D combustor computer program.

The assistance and guidance rendered by Dr. C. J. Marek, who was the NASA Project Manager for the program, is acknowledged.

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CHAPTER I

INTRODUCTION

A. Background

Significant advances have been made in combustor analytical modeling over the past five years. The use of advanced numerics and kinetics has given the combustion engineer the ability to predict internal combustor flow field characteristics. These advanced tools, while still in their incipient stages, offer the potential of reducing the design and development time required for gas turbine combustors. At the same time, the analytical models increase the understanding of the phenomena affecting combustor performance and provide the basis for designing better combustors. The optimization of the design process will require a judicious blend of the emerging analytical tools (correlated and updated with test data) with the established empirical techniques.

Starting in 1970, Garrett has demonstrated a company commitment to develop combustor analytical design tools and utilize them in the everyday design and development process. In addition to extensive company-sponsored efforts, a significant contribution to this highly successful effort has been the USARTL Combustor Design Criteria Validation Program (Contract DAAJ02-75-C-0044).[1] Among the models developed under the above-mentioned USARTL program was the 3-D Combustor Performance Model, which is the basis for the present program. The present program entailed extending the capability of the model to predict pollutant emissions of nitrogen oxides and smoke.

B. Objectives

The objective of the program was to utilize and extend an existing three-dimensional(3-D) combustor performance computer program:[1]

- To predict pollutant emissions of smoke and NO_x;
- To include the influence of soot, CO_2, and H_2O on radiation heat transfer; and
- To extend the two-step hydrocarbon oxidation mechanism to a more detailed four-step scheme.

The program consisted of four tasks:

- Task I - Formulation of the Method
- Task II - Computer Coding
- Task III - Computation of Test Cases
- Task IV - Reporting and Documentation.

In Task I, a method was formulated to predict the emissions of soot and NO_x and to extend the radiation and hydrocarbon oxidation models.

In Task II, the method was incorporated into the 3-D combustor program in order to compute the emissions of NO_x and soot and the radiant transfer to the combustor walls.

In Task III, the resulting program was exercised for idle, cruise, and takeoff conditions of a JT8D combustor.

In Task IV, reports were submitted to NASA during and at the end of the program.

C. Summary

This report is the Final Report of the computations of emissions program, and presents the work carried out by Garrett under the program. Chapter II of the report includes a brief description of the original 3-D combustor performance computer program, provided for completeness. Chapters III and IV describe the soot emissions model and the influence of soot on radiation heat transfer. The NO_x emissions model and the hydrocarbon oxidation mechanism are described in Chapters V and VI, respectively. Chapter VII includes a description of the results of the computations. Chapter VIII contains concluding remarks. Chapters IX and X, respectively, contain a list of nomenclature and list of references, as cited in this report. Finally, Appendices A, B, C, and D contain, respectively, a description of the 3-D program, the program input, a list of FORTRAN variables and a listing of the new 3-D combustor performance program.

CHAPTER II

DESCRIPTION OF THE 3-D COMBUSTOR PERFORMANCE PROGRAM

The 3-D Combustor Performance Model Computer Program that forms the basis of the present work, is briefly described. For complete details, refer to Report No. USARTL-TR-55C.[1]

The 3-D program is general and is capable of predicting recirculating turbulent flow in gas-turbine combustion chambers. Reacting or nonreacting, swirling or nonswirling, diffusion and/or premixed flames, and gaseous and/or liquid fuel combustion can be handled by the program. The program computes the following variables in the region of interest:

- Axial, radial, and swirl velocity components;
- Pressure;
- Enthalpy (temperature); in conjunction with the equation of state, the temperature determines the density variations in the flow field;
- Turbulent kinetic energy and its dissipation rate;
- Mass fractions of total fuel (mixture fraction), unburned fuel, oxygen, carbon monoxide, CO_2 and H_2O.
- Three radiation flux vectors;
- Spray trajectory, droplet size distribution, and evaporation rates.

The program employs the following physical models to solve the variables mentioned above:

- Turbulence - Two-equation ($k-\epsilon$) turbulence model to obtain turbulent kinetic energy and its dissipation rate.

- Chemistry - Two-step chemical reaction scheme:

$$C_xH_y + \left(\frac{x}{2} + \frac{y}{4}\right)(O_2 + nN_2) \rightarrow xCO + \frac{y}{2} H_2O + n\left(\frac{x}{2} + \frac{y}{4}\right) N_2 \quad (1)$$

$$CO + \frac{1}{2} O_2 \rightarrow CO_2 \quad (2)$$

- Chemical Reaction Rate - Fuel and CO consumption rates are assumed to be governed by either the time-averaged Arrhenius model or the turbulent eddy break-up model.

- Radiation - A six-flux model of radiation.

The transport equations for all dependent variables ϕ are written in the following general form:

$$\text{div}\left(\vec{\rho u}\phi - \frac{\mu_t}{\sigma_\phi} \text{grad}\ \phi\right) = S_\phi \quad (3)$$

where ρ denotes the mixture density, $\vec{u}$ the velocity vector, μ_t the effective or turbulent viscosity, σ_ϕ the effective Prandtl/Schmidt number, S_ϕ the sources of ϕ; i.e., S_ϕ includes the creation/destruction of ϕ plus other quantities that do not fall under the convective and diffusive terms. Table E-1 in Appendix E includes a list of the dependent variables ϕ and their source terms.

An iterative, general finite-difference solution procedure suitable for 3-D elliptic flows in complex geometries is used to solve the above system of coupled, nonlinear partial-differential equations. The solution procedure involves discretizing the differential equations by integration over elementary finite-difference control volumes surrounding grid nodes that are nonuniformly spaced over the flow field.

CHAPTER III

SOOT EMISSIONS

In this chapter, soot formation and oxidation in combustion chambers are discussed. A general background on soot emissions is provided first. Details of the soot formation and oxidation mechanisms reported in the literature are discussed next. Quasi-global expressions for soot formation and oxidation are described. A description of the influence of turbulence on soot formation and oxidation is included. The approach adopted in the present work is described next. This approach considers the influence of turbulent fluctuations on soot formation and oxidation rates.

A. Background

The particulate emission of primary concern in the combustion of hydrocarbon fuels is soot, which is evident in the form of exhaust smoke. The emission of smoke from gas turbine engines is responsible for the following problems:

- Higher liner temperatures due to increased radiative heat transfer
- Impingement of carbon on metal surfaces, resulting in erosion and reduced equipment lifetimes
- Distortion of fuel spray distribution due to carbon deposits, leading to hot spots
- Visible pollution and associated health hazards
- Tactical problems in military applications.

Recently, attention is being directed toward the combustion of alternate fuels derived from coal liquids and shale oil. Since the use of these fuels results in significant increases in smoke production, a better understanding of the physical and chemical processes governing soot production is needed.

The processes governing the formation and subsequent oxidation of soot are of a particularly complex nature; and, as such, quantitative models of soot production have yet to be developed. Soot is not an equilibrium product of combustion; and, therefore, its formation is influenced as much by the physical processes of atomization, evaporation, and fuel/air mixing as by reaction kinetics. Soot is generally produced anywhere within the combustor where fuel/air mixing is inadequate, resulting in oxygen-deficient, high-temperature zones.

For the pressures and temperatures normally prevalent in gas turbine combustors, equilibrium calculations indicate that solid carbon appears when there is insufficient oxygen to oxidize the hydrocarbon to CO and H_2 according to the relation:

$$C_xH_y + \frac{x}{2} O_2 \longrightarrow xCO + \frac{y}{2} H_2 \qquad (4)$$

That is, the carbon-oxygen mass ratio for incipient soot formation is 12:16; or, alternatively, the atomic C-O ratio is unity. However, since soot formation is essentially a nonequilibrium phenomenon, experimentally, soot is observed at C-O ratios (a) much less than unity at low temperatures ($\lesssim$2000°K); and (b) greater than unity at higher temperatures.[2]

Smoke levels are primarily dependent on the following:

- Air/fuel mixing
- Temperature

- o Equivalence ratio
- o Residence time of air/fuel mixture
- o Pressure
- o Fuel composition.

These factors influence both the formation and subsequent oxidation of soot and are dependent on engine operating conditions, details of the combustor internal flow field, fuel droplet characteristics, etc.

B. Mechanism of Soot Formation

Detailed discussions of the many mechanisms proposed to explain the chemical and physical processes governing soot formation are available in reviews by Haynes and Wagner,[3] Street and Thomas,[4] Palmer and Culliss,[5] Gaydon and Wolfhard,[6] Homann,[7] and Bittner and Howard.[8] Based on the information available, the process of soot formation can be considered to occur in three distinct stages:

- o Soot-particle nucleation
- o Agglomeration and surface growth
- o Coagulation.

The first stage of soot-particle nucleation is the most difficult to describe, and there is considerable controversy regarding this. The two most viable hypotheses advanced to date are based on ionic and radical polymerizations.

The theory of ionic polymerizations contends that positive ions serve as the nuclei for carbon formation in flames.[9,10] Based on this theory, Howard[11] showed that the chain structure of carbon particles and the uniform size of the spherical chain units can be explained. Experiments by Howard and coworkers[12] have demonstrated this theory to be feasible.

The theory of radical polymerizations considers that fuel pyrolysis gives rise to elementary unsaturated hydrocarbon molecules (e.g., acetylene), which polymerize via radical chain mechanisms.[13] Thus, soot formation is mainly due to gas-phase reactions and is not directly due to liquid pyrolysis. This mechanism has also been proposed by Porter[14] as the "Acetylene Mechanism of Soot Formation." Mass spectrometric measurements of species such as C_2H_2, C_4H_2, C_6H_2, C_8H_2, etc. obtained in flames[13] and shock-tube investigations[15] tend to support the radical polymerization theory. However, since a continuation of such a chain-reaction sequence cannot lead directly to carbon particles,[13] chain-branching and ring-closure, followed by agglomeration and dehydrogenation,[5,16] must take place at some point prior to soot formation.

In the second stage of soot formation (agglomeration and surface growth), spherical units of carbon particles (about 250Å in size) are formed by agglomeration and surface growth of the nuclei formed in the first stage.

Finally, in the third stage, the coagulation of the spherical carbon particles leads to the characteristic chain-like structure of soot. Dehydrogenation continues through both the second and third stages.

Jensen[17] proposed a model that treats the various steps of soot formation in some detail. The model agreed qualitatively with experimental observations in a methane flame. However, due to the complexities associated with the detailed reaction mechanism, and uncertainties in the rate constants, the Jensen model is not suitable for gas-turbine combustor analysis.

Since quantitative description of the soot formation mechanism applicable to general conditions are not available, quasi-global models as described later in this chapter are required for the computation of soot emissions.

C. Mechanism of Soot Oxidation

Analytical and empirical literature on soot oxidation is extensive. However, because of the complexities involved, considerable controversy exists concerning the mechanism of soot oxidation, and many basic questions have yet to be answered. Consideration of soot oxidation processes is important, since soot concentration in the exhaust gases is determined by both the relative rates of soot formation and oxidation in the flame zone and the surface oxidation rate in hot post-flame gases. In this Chapter, a limited review of the soot oxidation models and a rationale for selecting the model used in the present work is presented.

Many studies have been reported on the derivation of mass-transfer (oxidation) rates for single-carbon particles in a hot-oxidizing ambient environment. Recently, studies on the theory of burning carbon particles were made by Avedesian and Davidson,[19] Ubhayakar and Williams,[20] and Libby and Blake.[21] These studies involved simplifying assumptions with regard to the fluid-mechanical and chemical aspects of the problem. Amundson and coworkers[22,23,24] presented a model for the diffusion and chemical reaction in the boundary layer surrounding a burning spherical carbon particle in a quiescent gas. The model accounted for radiation and for the homogeneous combustion of CO in the gas phase and the heterogeneous surface reactions of carbon with oxygen and CO_2. The model predicted the distribution of the product concentrations around the particle.

High-temperature soot oxidation rates were measured by Lee, et al.,[25] in the tail of propane diffusion flames. The soot oxidation rate (R_{ox}) per unit particle surface area was determined as a function of temperature and partial pressure of oxygen, as follows:

$$R_{ox}=1.09\times10^{5}P_{O_2}T^{-1/2}\exp(-19725/T)\ kg/m^2s \qquad (5)$$

The measurements were conducted in the temperature range of 1310° to 1670°K. Tesner and Tsibulevsky[26] also measured flame-soot oxidation rates over the temperature range of 1400° to 2000°K and found good agreement with the above expression. Feugier[27] measured soot concentrations in fuel-rich ethane-oxygen flames and deduced a kinetic expression for the oxidation of soot particles similar to the one by Lee, et al.[25]

Based on the measurements of the surface oxidation rates of pyrolytic graphite and the similarity of small soot particles to pyrolytic graphite at the microscopic level, Radcliffe and Appleton[28] proposed that the soot oxidation rate should exhibit a local maximum (for a fixed O_2 partial pressure and increasing temperature) at temperatures from 2000° to 2500°K for O_2 partial pressure in the range of 0.05 to 1.0 atmosphere. Additionally, the soot oxidation rate should exhibit a first-order dependence on the O_2 partial pressure for $P_{O_2} \leq 0.01$ atmosphere and, at higher pressures, should asymptotically approach a zero-order dependence. The semi-empirical formula for soot oxidation rate proposed by Nagle and Strickland-Constable[29] (discussed later in this chapter) confirms this behavior. The model of Lee, et al., can be derived from that of Nagle and Strickland-Constable for fuel-lean conditions. Therefore, the more general model of Nagle and Strickland-Constable has been adopted in the present work.

D. Quasi-global Models of Soot Formation and Oxidation

Since the elementary steps in the formation and oxidation of soot are not totally understood, the present program uses quasi-global models that characterize soot production occurring via a few overall steps. Such models have been successful in predicting soot production.[32] In this section, some of the quasi-global models reported in the literature are described.

The quasi-global models do not predict the size of soot particles. With the current state-of-the-art, it is not possible to predict the size of formation of the soot particles in any practical flow situation. Therefore, it is assumed that particles are produced at a known size. It may also be assumed that particles are produced in accordance with a specified size distribution (e.g., Gaussian).

Tesner, et al.,[33] proposed a soot production model which grouped the complex processes of pyrolysis, nuclei formation, and soot formation into three rate-limited subglobal steps that include (a) a pyrolysis rate first order in hydrocarbon concentration, (b) a chain branching and chain termination rate for soot nuclei formation rate, and (c) a soot formation rate.

Pyrolysis:

$$n_o = a_o C_{fu} \exp(-E/RT) \quad (\text{part.}/\text{m}^3.\text{s}) \tag{6}$$

Nuclei Formation:

$$R_{n,f} = n_o + (f-g)n - g_o Nn \quad (\text{part.}/\text{m}^3.\text{s}) \tag{7}$$

Soot Formation:

$$R_{S,f} = m_p (a - bN) n \quad (\text{kg}/\text{m}^3.\text{s}) \tag{8}$$

where a_o, E, f, g, g_o, a, and b are constants for a given fuel; n_o is the rate of spontaneous formation of nuclei; n is the nucleus concentration; N is concentration of soot particles; m_p is the mass of a soot particle; and $R_{n,f}$ and $R_{S,f}$ are the nuclei and soot formation rates, respectively.

Khan and Greeves[34] proposed a single-step global expression as a function of the partial pressure of unburned hydrocarbons (P_{HC}), the unburned equivalence ratio (ϕ_u), and the temperature (T):

$$R_{S,f} = 0.468\ P_{HC}\ \phi_u^3\ \exp\ (-40{,}000/RT)\quad gm/cm^3s \tag{9}$$

This model is overly sensitive to the equivalence ratio and, therefore, is not considered in the present work. In addition, in both the above models, soot oxidation rates are not considered.

Edelman, et al.,[32] consider both soot formation (R_f) and soot oxidation (R_{ox}) and express the net soot formation rate as:

$$\frac{dC_s}{dt} = R_f - A_t R_{ox} \tag{10}$$

where A_t equals total surface area available for oxidation. This model is more general and, therefore, it has been adopted in the present work with appropriate modifications to account for turbulence effects as described next in Section E. The formation step is expressed by a modified Arrhenius type of relation:

$$R_f = AT^{\alpha} C_{HC}^{a}\ C_{O_2}^{b}\ \exp\ (-E/RT)\ gm/cm^3s \tag{11}$$

where C_{O_2}, C_{HC} equal the concentration of unburned oxygen and hydrocarbon (gm/cm^3) and where A, α, a, b, E are model constants.

For the oxidation step, Edelman, et al.,[32] adopt the semi-empirical formula of Nagle and Strickland-Constable[29] for pyrolytic graphite oxidation; this formula is nonlinear and non-Arrhenius in P_{O_2} and T:

$$A_t R_{OX} = 12\left[\left(\frac{K_A P_{O_2}}{1+K_Z P_{O_2}}\right)\psi + K_B P_{O_2}(1-\psi)\right] A_t \text{ gm/s} \qquad (12)$$

where:

$$\psi = [1 + K_T/(K_B P_{O_2})]^{-1} \qquad (13)$$

$$K_A = 20 \exp(-30{,}000/RT) \text{ gm/cm}^2\text{.s atm} \qquad (14)$$

$$K_B = 4.46\times10^{-3} \exp(-15{,}200/RT) \text{ gm/cm}^2\text{.s. atm.} \qquad (15)$$

$$K_T = 1.51\times10^{5} \exp(-97{,}000/RT) \text{ gm/cm}^2\text{.s} \qquad (16)$$

$$K_Z = 21.3 \exp(4100/RT) \text{ atm}^{-1} \qquad (17)$$

Shock-tube measurement[18] of soot oxidation rates qualitatively confirms the features of the above formula. With these expressions for soot formation and oxidation and assuming a single-soot particle size of 250Å, Edelman, et al.[32] obtained close agreement of the predicted soot concentration (mg/l) with the experimental data in a jet-stirred reactor. Thus, these expressions assume perfect mixing. In a gas-turbine combustor, however, regions of unmixed species will exist, and turbulence will also influence the soot production rates. As such, modifications to these expressions are required before they can be used for a general 3-D turbulent flow.

E. Influence of Turbulence on Soot Formation and Oxidation

Magnussen, et al.,[35,36] have proposed a model that accounts for the influence of turbulent fluctuations on soot production rates.

In turbulent flows, chemical reaction occurs when reactants at a sufficiently high temperature are mixed at the molecular level. The molecular mixing process is analogous to the dissipation (ϵ) of turbulent kinetic energy k and is associated with the smallest scales of turbulence. Dissipation is concentrated in highly strained regions of the fluid occupied by fine structures with characteristic dimensions of the same magnitude as the Kolmogorov microscale. The reactants are molecularly mixed in these fine structures, where reaction occurs. Magnussen, et al., proposed the following expressions for the mass fraction contained in the fine structures:

$$\gamma^* = 9.7 \cdot (R_t)^{-3/4} \tag{18}$$

where R_t is the turbulence Reynolds number, and the rate of transfer of mass per unit mass between the fine structures and the surrounding fluid is:

$$\dot{m} = 23.6 \cdot (R_t)^{-1/4} \frac{\epsilon}{k} \tag{19}$$

The rate of reaction is proportional to $\dot{m}\chi$ where χ is the fraction of small-structure eddies that are sufficiently heated to react. It is assumed that χ is proportional to the ratio of local reacted fuel concentration and total fuel concentration. Thus, the rate of reaction is:

$$R_{fu} = 23.6 \ (R_t)^{-1/4} \frac{\epsilon}{k} \chi \quad C_{min} \ _{(kg/m^3 \ s)} \tag{20}$$

where

$$\chi = \frac{C_{pr}/(1 + i)}{C_{pr}/(1 + i) + C_{fu}} \tag{21}$$

C_{min} is the smaller of C_{fu} and (C_{O_2}/i) and i is the stoichiometric oxygen requirement. The temperature T* of the reacting fine structures is T above the local time-mean temperature T:

$$T^* = T + \Delta T = T + \frac{\Delta H_R}{\rho C_p} C_{min} \tag{22}$$

where

ΔH_R = the heat of reaction
C_p = the specific heat

and the surrounding temperature T^o is

$$T^o = T - \Delta T \frac{\gamma^* \chi}{1 - \gamma^* \chi} \tag{23}$$

Using Equations (6) and (8), the mean rates of nuclei and soot formation are then expressed as:

$$R_{n,f} = n_{o,T^*} \gamma^* \chi \rho/\rho^* + n_{o,T^o} (1 - \gamma^* \chi) \rho/\rho^o$$

$$+ (f - g) n - g_o n^* N^* \gamma^* \chi \rho/\rho^*$$

$$- g_o n^o N^o (1 - \gamma^* \chi) \rho/\rho^o \tag{24}$$

and

$$R_{s,f} = m_p (a - b N^*) n^* \gamma^* \chi \rho/\rho^* + m_p (a - b N^o) n^o$$

$$(1 - \gamma^* \chi) \rho/\rho^o$$

Finally, the mean rates of nuclei and soot oxidation are expressed as:

$$R_{n,c} = R_{fu} n/C_{fu} \text{ (part/m}^3 \text{ s)} \tag{26}$$

$$R_{s,c} = R_{fu} C_s/C_{fu} \text{ (kg/m}^3 \text{ s)} \tag{27}$$

Magnussen, et al., used this model to compute the soot concentrations in a turbulent C_2H_2 diffusion flame. By adjusting the particle diameter [entered as m_p, the particle mass in Equation (8), and the constant a_o in Equation (6), good agreement with experimental measurements was obtained.

F. Present Approach

The model adopted for computing soot emissions in the present program is described in the following paragraphs.

The computation of soot emissions involves the solution of two additional transport equations for the concentrations of (a) nuclei and (b) soot. These two equations are of the same general form as Equation (3) solved by the 3-D Combustor Program. To complete the equation specifications, the source terms and the Schmidt numbers for these two variables are as follows:

The source term in the nuclei concentration equation is expressed as

$$R_{n,f} - R_{n,c} \tag{28}$$

where $R_{n,f}$ is given by the smaller of the two values from Equations (7) and (24); $R_{n,c}$ is given by Equation (26). Thus, these expressions amount to the use of the turbulent reaction rates, subject to the limitation that they cannot be greater than the rates under well-stirred reactor conditions.

The source term in the soot concentration equation is similarly expressed as

$$R_{s,f} - R_{s,c} \tag{29}$$

where $R_{s,f}$ is given by the smaller of the two values from Equations (11) and (25); $R_{s,c}$ is given by the smaller of the two values from Equations (12) and (27).

The turbulent Schmidt numbers σ_s and σ_n for soot and nuclei concentrations are assumed the same as for gaseous fuel (i.e., 0.9).

In the computations carried out in the present work, a distribution of two particle sizes was considered: a small size of 0.025 microns as resulting from nucleation and a large size of one micron as resulting from fuel droplet pyrolysis and char formation. The relative rates of formation of these two sizes of particles was assumed to be 90-10 percent. The consideration of two particle sizes leads to the solution of a transport equation of the same general form as Equation (1) for the concentration of the particles in each size. The extension to other sizes is straightforward but involves extra computational effort, since an additional equation must be solved for each additional size considered. In view of the several assumptions inherent in the analysis of soot production, the consideration of other size groups is not necessary at this stage.

The calculation of soot formation is bypassed if the temperature is less than a value below which the formation rates are negligible. It is also bypassed if the local carbon-to-oxygen ratio is less than the incipient soot formation limit. Both of these limits of temperature and carbon-to-oxygen ratio are inputs to the calculation procedure and can be varied at will.

A lack of data exists for computing particle coagulation. Attempts to model particle growth in flames[38,39] have had little success. No definite conclusions could be reached with these models. A lack of understanding of the phenomena and the absence of data reduces coagulation computations to mere speculation. Therefore, this phenomenon is not addressed in the present work.

CHAPTER IV

RADIATION HEAT TRANSFER

A. Background

The contributors to radiation in combustors fueled by hydrocarbons are soot, CO_2, H_2O (vapor), inorganic particles, CO, unburned fuel (C_xH_y), NO_x, and SO_2. Only the influence of soot, CO_2, and H_2O (vapor) are considered in the present work. Although CO and unburned C_xH_y contribute to emission and attenuation of radiation within flames, these contributions are localized and of secondary importance when total heat-transfer rates are considered. The contributions of NO_x and SO_2 can be neglected because of their low concentrations.

The determination of the influence of soot on radiant heat transfer reduces to two factors: (a) soot distribution in the flame and (b) the radiative properties of gas-soot mixtures. The first was discussed in the preceding chapter. Radiative properties of gas-soot mixtures are discussed in this chapter.

The radiation properties of the principal radiating species including soot, CO_2, and H_2O, are significantly nongrey. Consequently, the calculation of the radiation properties is a time-consuming task. However, spectral calculations are unnecessary since approximate calculations (by means of curve fits) are more convenient and provide good accuracy.[40]

An approximate curve-fit procedure for the calculation of radiation properties is employed in the present work.

B. Radiation Properties of Soot, CO_2, and H_2O Mixtures

The absorptivity (α) of the gas-soot mixture includes the soot absorptivity, the absorptivity due to the absorption bands of CO_2 and H_2O, and corrections for the overlapping of bands.

Utilizing the spectral data,[41] the gas absorptivity is calculated by taking a summation over the absorption bands of CO_2 and H_2O. In the approximate calculation method adopted here, a simpler approach is used. The gas absorptivity α_g is written as[42]

$$\alpha_g = \epsilon_g \, (T/T_s)^{(0.6-0.2\zeta)} \tag{30}$$

where $$\zeta = P_w/(P_w+P_c) \tag{31}$$

ϵ_g = gas emissivity at a temperature T and path length LT_s/T

T, T_s = gas and blackbody source temperatures, respectively

P_c, P_w = partial pressures of CO_2 and H_2O

ϵ_g is given by

$$\epsilon_g = \epsilon_c + \epsilon_w - \Delta\epsilon_{cw} \tag{32}$$

where ϵ_c, ϵ_w = emissivities of CO_2 and H_2O

$\Delta\epsilon_{cw}$ = overlap correction factor

ϵ_g can be computed using a temperature adjusted version of Leckner's[43] approximate overlap correction $\Delta\epsilon_{cw}$, and approximating

ϵ_c and ϵ_w by curve fits of Pc, Pw, PL, and T to spectral calculations. In the range of interest in gas-turbine combustors, such calculations agree to within 5 percent of the spectral calculations and the experimental results.

The temperature adjusted version of Leckner's[43] overlap correction $\Delta\epsilon_{cw}$, which accounts for the 2.7 and 15μm overlapped regions for mixtures of CO_2 and H_2O, is[40]

$$\Delta\epsilon_{cw} = \frac{\zeta}{(10.7 + 101\zeta)} - \frac{\zeta^{10.4}}{111.7}$$

$$\{\log_{10}[101.3(P_c + P_w)L]\}^{2.76} F(T)$$

$$\text{for } (P_c + P_w)L \geq 0.1 \text{ atm-m}$$

$$= 0 \text{ for } (P_c + P_w)L < 0.1 \text{ atm-m}$$

where ζ is defined by Equation (31) and F(T) is given by:

$$F(T) = -1.0204 \times 10^{-6}T^2 + 2.2449$$

$$10^{-3}T - 0.23469 \quad (T \text{ in degrees K})$$

The coefficients involved in the curve fits of ϵ_c and ϵ_w to P_c, P_w, PL and T are given in Reference 40 and are not reproduced here.

The absorptivity (α) of the gas-soot mixture is given by

$$\alpha = \alpha_s + \alpha_g - \alpha_s\alpha_g \tag{33}$$

With α_g obtained above, it remains to determine α_s, the soot absorptivity. This is obtained by the method of Felske and Tien.[44] This method assumes that the complex refractive index of soot is independent of wavelength and that the soot particle diameter is small compared to the wavelength of radiation, so that scattering is negligible. The spectrally integrated absorptivity α_s can then be written in a closed-form expression to determine α_s.

By using the radiative property calculations of the type described above, Sarofim[45] indicated that radiation calculations can be made with fair confidence, and that the major source of uncertainty in such calculations is soot concentration, rather than gas-radiation properties.

C. Present Approach

The six-flux radiation model incorporated into the 3-D Combustor Performance Computer Program was used in computing radiation heat transfer in the present work.

This model is based on the Schuster-Hamaker approximation.[46] It should be noted that, as pointed out by Siddall,[47] other flux model approximations such as Milne-Eddington and Schuster-Schwarzschild can be represented by the same form of flux equations with constants being different.

The differential equations describing the variations of the fluxes along six directions can be reduced to the following three second-order ordinary differential equations:

$$\frac{d}{dx}\left(\frac{1}{a+S}\frac{dR^x}{dx}\right) = a\,(R^x-E) + \frac{S}{3}\,(2R^x - R^r - R^z) \tag{34}$$

$$\frac{1}{r}\frac{d}{dr}\left(\frac{r}{a+S+\frac{1}{r}}\frac{dR^r}{dr}\right) = a(R^r-E) + \frac{S}{3}\,(2R^r - R^x - R^z) \tag{35}$$

$$\frac{1}{r}\frac{d}{d\theta}\left(\frac{1}{a+S}\frac{dR^z}{r\,d\theta}\right) = a(R^z - E) + \frac{S}{3}\,(2R^z - R^x - R^r) \tag{36}$$

Where the composite-fluxes R^x, R^r and R^z are defined as

$$R^x = \frac{1}{2}\,(I_{x+} + I_{x-}) \tag{37}$$

$$R^r = \frac{1}{2} (I_{r+} + I_{r-}) \tag{38}$$

$$R^z = \frac{1}{2} (I_{\theta+} + I_{\theta-}) \tag{39}$$

where I_{x+}, I_{r+}, and $I_{\theta+}$ are the fluxes along the positive directions of axial, radial, and circumferential directions, respectively; I_{x-}, I_{r-}, and $I_{\theta-}$ are the corresponding fluxes along the negative directions.

a = Absorption coefficient, defined as radiation absorbed per unit length

S = Scattering coefficient, defined as radiation scattered per unit length

E = Black body emissive power = σT^4

σ = The Stefan-Boltzman constant

The absorption coefficient a is related to the absorptivity α of the gas-soot mixture and the path length L by:

$$a = -\frac{1}{L} \ln (1-\alpha)$$

In the original version of the 3-D combustor program,[1] the radiation properties were assigned constant values. For the present work, the absorption coefficient was computed locally as a function of gas and soot concentrations by the approximate procedure described above.

The scattering due to soot particles, which are generally of diameters below one micron, is negligible. In the present work, a uniform value of $0.01 m^{-1}$ was assumed for the scattering coefficient.

CHAPTER V

NITROGEN-OXIDE EMISSIONS

A. Background

Nitrogen oxides (NO_x) are formed during any combustion process involving air within the normal range of adiabatic flame temperatures and comprise nitric oxide (NO), nitrogen dioxide (NO_2), and small amounts of nitrous oxide (N_2O). For turbopropulsion engines, the NO_x emissions consist mostly of NO, particularly at high power conditions, where maximum NO_x concentrations are encountered. However, the contribution of NO to total NO_x emissions decreases at low power points. The NO_x is conventionally expressed in mass units of NO_2, to which the NO would eventually react in the atmosphere.

The major influences contributing to the formation of NO_x are (a) high flame temperature, (b) the availability of oxygen as provided by excess air, and (c) sufficient residence time for the reactions to take place. Formation of NO is preceded by the generation of N and O atoms. Nitrogen (N) atoms are formed by the dissociation of nitrogen (N_2) in the air at high temperatures, and can also be a product of hydrocarbon reactions if the fuel contains nitrogen. Oxygen (O) atoms are formed primarily from oxygen (O_2) dissociation. Thus, NO forms both in the reaction zone and in the post-reaction, high-temperature gases. A super-equilibrium of O, N, and OH concentrations (i.e., concentrations exceeding equilibrium levels) in the reaction zone leads to NO formation in this zone (often termed as 'prompt NO'). Nitric oxide formation is controlled by rate-limited reactions, and its calculation is dependent on a knowledge of other radical concentrations.

The conservation equations for the radical and NO_x concentrations form a set of coupled 'stiff' nonlinear differential equations and their solution requires special integration procedures. One such procedure, which has been developed by Pratt and Wormeck,[48] is described next. This procedure has been incorporated into the 3-D combustor program and has been used to compute the NO_x emissions in the present work.

B. The Chemical Kinetics Program

The conservation equations for the species involved in NO_x production form a set of 'stiff' equations. Pratt and Wormeck[48] have developed a numerically efficient computer program (CREK) for the solution of such a set of equations. The CREK procedure is briefly described in the following paragraphs.

The species and energy conservation equations for a node, P, are expressed in the following standard finite-difference form:

$$A_P\phi_P = A_E\phi_E + A_W\phi_W + A_N\phi_N + A_S\phi_S + A_H\phi_H + A_L\phi_L + S_\phi \qquad (40)$$

where A is the finite-difference coefficient containing the convective and diffusive fluxes; ϕ is the dependent variable (species concentration, enthalpy); S_ϕ is the source of ϕ; subscripts E, W, N, S, H, and L refer to the six neighboring nodes of P.

The CREK program is used to solve the above finite-difference equation. The solution is simultaneous for all the species concentrations and temperature at a given node P; and proceeds node-by-node until all of the nodes in the flow field are covered. The solution procedure involves the derivation of a set of Newton-Raphson correction equations for the species concentrations and temperature. These equations are solved iteratively by pivoted Gaussian elimination.

The program requires as input the following information:

(1) Previous solution or estimate of ϕ_P and temperature at node P;

(2) Pressure at node P;

(3) Finite-difference coefficients A_P A_E, A_W, A_N, A_S, A_H, and A_L, as calculated in the 3-D combustor program;

(4) $\phi_P^* = (A_E\phi_E + A_W\phi_W + A_N\phi_N + A_S\phi_S + A_H\phi_H + A_L\phi_L)/A_P$

(5) Enthalpy source coeffients Q, where, enthalpy source = $-(Q_0 + Q_1T + Q_2T^2 + Q_3T^3 + Q_4T^4)$.

The outputs from the program are

(1) Mole numbers of all chemical species;

(2) Temperature at node P;

(3) Density at node P.

Further details of the CREK procedure are contained in Reference 48.

C. Present Approach

The number of species considered in the present program is 14: C_xH_y, C_xH_{y-2}, CO, CO_2, H, H_2, O, O_2, OH, H_2O, N, N_2, NO, NO_2. Here, C_xH_{y-2} denotes the intermediate hydrocarbon as explained in Chapter VI. Each of these species concentrations is governed by a transport equation of the same general form as Equation (3). To complete the equation specifications, the source terms and the

Schmidt numbers for these variables have to be determined. The turbulent Schmidt numbers, σ_ϕ, for all the species are assumed to be 0.9. The computation of the source terms, S_ϕ, is based on the reaction mechanism given in Table I. The calculation involved for each reaction is illustrated below with reference to the reaction A+B $\rightleftharpoons$ C+D.

The laminar Arrhenius rate

$$R_L = \rho^2 M_A M_B \, A T^b \exp(-E/RT) \tag{41}$$

where M_A and M_B are the mass fractions of A and B.

The turbulent eddy-break-up rate for species A is

$$R_T = C_R \rho M_{MIN} \, \epsilon/k \tag{42}$$

where C_R is a constant, ρ is the density, and where M_{MIN} is the smaller of M_A and M_B/i, i being the mass of B required per unit mass of A in this reaction. The rate of production/consumption of A is

$$R = \text{smaller of } R_L \text{ and } R_T$$

The backward rate is treated similarly. All of the reactions listed in Table I and the global reactions discussed in Chapter VI are treated in this way, and the sources due to chemical reaction in the conservation equations for the species are obtained by summing the rates due to all of these reactions. The resulting species equations are solved by the computer program CREK described above. This determines the concentrations of all of the species. Modifications have been made to the CREK program in the present work in order to treat the global reactions and the eddy-break-up rates for the reaction steps.

TABLE I. NO_x REACTION MECHANISM.

$$K_f = 10^x T^b \exp(-E/RT)$$

	Reaction							X	b	E/R (°K)
1.	H	H	M	=	H2		M	12.300	-1.000	0.0
2.	O	O	M	=	O2		M	11.000	-1.000	0.0
3.	H	OH	M	=	H2O		M	13.850	-1.000	0.0
4.	H	O2		=	OH	O		11.350	0.0	8400.000
5.	O	H2		=	OH	H		10.240	0.0	4730.000
6.	H	H2O		=	OH	H2		10.920	0.0	10050.000
7.	O	H2O		=	OH	OH		10.760	0.0	9000.000
8.	N2	O		=	NO	N		9.000	0.0	25000.000
9.	N	O2		=	NO	O		5.000	1.000	2000.000
10.	N	OH		=	NO	H		9.000	0.0	0.0
11.	N2	O2		=	N	NO2		11.431	-1.000	60600.000
12.	NO	NO		=	N	NO2		7.000	0.0	0.0
13.	NO	O2		=	NO2	O		9.000	0.0	22900.000
14.	H	NO2		=	NO	OH		10.477	0.0	0.0

NOTE: Values are in SI units.
Reverse rate constant obtained from forward rate constant equilibrium constant.

The consideration of a detailed mechanism as shown in Table I is computationally time consuming when considering a three-dimensional problem. The chemical kinetics solution involves a point-by-point procedure, proceeding from one grid node at a time to the next until all nodes are covered. At any stage, the species concentrations at the nodes that are yet to be solved also influence the concentrations at the node currently being solved. Therefore, the concentrations at the nodes not yet solved, have to be estimated or are known from the previous iteration. Due to this explicit (as opposed to implicit) nature of the coupling between values at neighboring nodes, the solution has to be repeated several times in order to achieve convergence with attendent large computer times.

In order to reduce computer times, the partial equilibrium assumption has been used in some work reported in the literature. This involves the assumption that the following four bimolecular reactions are equilibrated:

$$H + O_2 \rightleftharpoons OH + O \quad (43)$$

$$O + H_2 \rightleftharpoons OH + H \quad (44)$$

$$OH + OH \rightleftharpoons H_2O + O \quad (45)$$

$$CO + OH \rightleftharpoons CO_2 + H \quad (46)$$

This assumption reduces the number of kinetic equations to be solved. The equilibration of these reactions in several premixed combustion systems is supported by the studies of References 49-51. Their equilibration in a CH_4-Air diffusion flame was demonstrated by Mitchell, et al.[25] They showed that these reactions are in equilibrium over a range of equivalence ratios from little less than unity up to approximately 2.5 for a flame at atmospheric pressure with the reactants initially at about 300°K. The equilibration of these reactions at different conditions, more closely resembling those in gas-turbine combustors, has not been demonstrated. Thus,

the partial equilibrium assumption may not be valid in all regions of a gas-turbine combustor; hence, it has not been used in the present work. The present approach, although more time-consuming, is general and does not involve any simplifications regarding the chemistry.

There have been reports of fast integrators for stiff kinetic equations in recent literature, e.g., Reference 57. The use of these instead of CREK (which was used in the present work because of its availability in a well-tested form while other schemes were still in their development and testing phases) will reduce computer times and will make fine grid 3-D computations possible without undue computational costs. The framework for the kinetics calculations has been provided here and the substitution of CREK for another procedure should be a straightforward task. The use of fast integrators will also enable the treatment of a more detailed reaction mechanism for NO_x. Thus, steps involving species such as HCN (on fuel-rich side) can be included if reliable kinetic data is available.

CHAPTER VI

THE FOUR-STEP HYDROCARBON OXIDATION MECHANISM

A. Background

A successful modeling of combustion systems depends on an adequate description of the reaction mechanism. For hydrocarbon oxidation, a large number of species participating simultaneously in numerous elementary kinetic steps is required to specify the reaction mechanism. This results in "stiff" differential equations requiring special time-consuming integration methods. For a complex 3-D problem, the computing costs would be prohibitive. Besides the large number of species equations to be solved, the elementary steps and their rate constants are not well known except for the simplest of hydrocarbons e.g., CH_4. To get around this problem, the gas turbine combustion modeling effort has frequently been simplified by using a global approach that reduces chemistry to the specification of an overall global oxidation scheme, which can predict quantities of interest: fuel consumption and heat release rates.

The oxidation of hydrocarbon fuel can be described by the following basic steps:

(a) Transformation of the hydrocarbon fuel into intermediate hydrocarbons and hydrogen with little release of energy;

(b) Oxidation of intermediates to CO and H_2;

(c) Oxidation of CO to CO_2;

(d) Oxidation of H_2 to H_2O.

Steps (b) through (d) are exothermic and are responsible for the release of energy and associated temperature rise. A global reaction scheme, which is designed to correctly model the oxidation process, must include a description of these steps.

B. Hydrocarbon Reaction Mechanisms

One Step Scheme

The simplest global mechanism is the one-step scheme:

$$C_X H_y + (X + \tfrac{y}{4})\ O_2 \rightarrow XCO_2 + \tfrac{y}{2}\ H_2O \qquad (47)$$

The advantage of this mechanism is its simplicity; it involves the solution of the conservation equations for unburned fuel and the mixture fraction. The heat release and the concentrations of the other species are then obtained from linear functions of the amount of fuel consumed. This mechanism, however, fails to predict the important characteristics of hydrocarbon oxidation, i.e., the formation of intermediates and CO, which influence the process considerably. As a result, this mechanism is inadequate for obtaining quantitative predictions.

Two-Step Scheme

A slightly more complex scheme is the two-step mechanism:

$$C_X H_y + (\tfrac{X}{2} + \tfrac{y}{4})\ O_2 \rightarrow XCO + \tfrac{y}{2}\ H_2O \qquad (48)$$

$$CO + \tfrac{1}{2}\ O_2 \rightarrow CO_2 \qquad (49)$$

This involves the solution of one additional equation: that for the concentration of CO. Here again, the formation of intermediates is ignored and so this mechanism cannot predict the time delay

between the initial disappearance of fuel into intermediates and a significant rise in temperature.

Four-Step Scheme

The simplest mechanism which accounts for the essential features of the hydrocarbon oxidation is the following four-step scheme proposed by Hautman, et al.[53]

$$C_N H_{2N} + 2 \rightarrow \frac{N}{2} C_2 H_4 + H_2 \quad (50)$$

$$C_2 H_4 + O_2 \rightarrow 2CO + 2H_2 \quad (51)$$

$$CO + 1/2\ O_2 \rightarrow CO_2 \quad (52)$$

$$H_2 + 1/2\ O_2 \rightarrow H_2O \quad (53)$$

This scheme is valid only for aliphatic hydrocarbons of the type $C_N H_{2N+2}$. To accommodate a general hydrocarbon $C_X H_y$, the first two steps have been modified in the present work:

$$C_X H_y \rightarrow C_X H_{y-2} + H_2 \quad (54)$$

$$C_X H_{y-2} + \frac{X}{2} O_2 \rightarrow X\ CO + \frac{y-2}{2} H_2 \quad (55)$$

This scheme involves the solution of two additional equations: for the concentrations of $C_X H_{y-2}$ and H_2.

The rate expressions for the four-step scheme developed primarily from propane oxidation results[53] are

$$\frac{d[C_X H_y]}{dt} = -10^x \exp(-E/RT)[C_X H_y]^a [O_2]^b [C_X H_{y-2}]^c \text{ mole/cc-s} \quad (56)$$

$$\frac{d[C_xH_{y-2}]}{dt} = -10^x \exp(-E/RT)[C_xH_{y-2}]^a[O_2]^b[C_xH_y]^c \text{ mole/cc-s} \quad (57)$$

$$\frac{d[CO]}{dt} = \left\{-10^x \exp(-E/RT)[CO]^a[O_2]^b[H_2O]^c\right\} \times S \text{ mole/cc-s} \quad (58)$$

$$\frac{d[H_2]}{dt} = -10^x \exp(-E/RT)[H_2]^a[O_2]^b[C_xH_{y-2}]^c \text{ mole/cc-s} \quad (59)$$

where [CO], etc. are the species concentrations in gm-moles/cc. The parameters[53] for (56) are x = 17.32 ±0.88, E = 49,600 ±2400, a = 0.50 ±0.02, b = 1.07 ±0.05, and c = 0.40 ±0.03;

for (57), x = 14.70 ±2.00, E = 50,000 ±5000, a = 0.90 ±0.08, b = 1.18 ±0.10, and c = -0.37 ±0.04;

for (59), x = 13.52 ±2.2, E = 41,000 ±6400, a = 0.85 ±0.16, b = 1.42 ±0.11, and c = -0.56 ±0.20;

and for (58), x = 14.6 ±0.25, E = 40,000 ±1200, a = 1.0, b = 0.25, and c = 0.50;

S = 7.93 exp(-2.48ϕ), where ϕ is the initial equivalence ratio and S cannot take values greater than 1.

The rate expressions were found to predict within reasonable accuracy flow reactor and shock tube results on propane oxidation, which encompass an equivalence ratio range 0.12 to 2.0, a temperature range 960 to 1540K, and a pressure range 1 to 9 atm. With modification to the parameters, experimental flow reactor results on the oxidation of butane, 2- and 3-methylpentane, and n-octane are also predicted.[53]

The tolerance bands on the various parameters reflect the sensitivity of the predictions to these parameters and the modifications necessary to the values of these parameters in order to

obtain predictions in agreement with experimental measurements for different conditions. In the present work, it was found that the tolerance band on most of the parameters is rather wide and that for any given flow, changing a parameter from its lower to its upper limit can alter the predictions significantly. For the results reported in Chapter VII, the median values of all the parameters were used. Further comparison with more experimental measurements is necessary in order to narrow the tolerance bands and obtain more certain values.

C. Present Approach

The four-step mechanism described above has been incorporated into the 3-D Combustor Performance Program. This involved the solution of two additional differential equations of the same general form as Equation (3), for the concentrations of C_xH_{y-2} and H_2. The source terms in these equations were obtained from the mechanism given by Equation (50-55). The rate expressions given by Equations (56-59) were modified by the eddy-break-up rate to account for the influence of turbulence. The procedure used was the same as that for the fuel equation[1]. The effective Schmidt numbers for these two species were assumed to be the same as for other species, i.e., 0.9.

Other modifications to the 3-D program to incorporate the four-step scheme were:

- The source terms for C_xH_y and CO were modified to be in accordance with the four-step scheme: C_xH_y consumed in Step (1); CO produced in Step (2) and consumed in Step (3).

- Mixture molecular weight, density, enthalpy (and hence temperature) calculation sequences were modified to include the two new species: C_xH_{y-2} and H_2.

- Computations of O_2, CO_2, H_2O concentrations from element conservation were modified to include the two new species: C_XH_{Y-2} and H_2.

The four-step scheme was proved to be far superior to the two-step scheme in computations of a plug flow reactor (see Chapter VII, Results).

CHAPTER VII

RESULTS AND DISCUSSION

In this section, the results of the computations performed in the present program are described. The results of the validation of the four-step hydrocarbon oxidation scheme are presented followed by computations of the emissions from a JT8D combustor.

A. Four-Step Hydrocarbon Oxidation Scheme Results

Measurements in a plug flow reactor were conducted by Hautman, et al.,[53] for lean, stoichiometric, and rich propane flames. These measurements were used to test the validity of the four-step scheme. Computations were performed for these three cases with both the two-step and four-step schemes. Sixty axial grid points were used in these computations. Reduction of the axial spacing by a factor of two, showed negligible changes, thus demonstrating the grid-independency of the results.

Comparison of the results with the measurements are shown in Figures 1, 2, and 3 for the lean, stoichiometric and rich cases, respectively. From these figures, it is clear that the four-step scheme is far superior to the two-step scheme in predicting the salient features of hydrocarbon combustion.

Figure 1 (a, b, and c) shows the two-step and four-step hydrocarbon oxidation scheme predictions and the corresponding measurements for the lean C_3H_8 flame. The four-step predictions of CO_2, C_3H_8, and temperature agree very closely with the measurements. The four-step CO and H_2 predictions are slightly higher than the measurements, but the discrepancy is not large. Since in the predictions all the intermediates are lumped into C_2H_4, the total measured intermediates are shown in Figure 1c for a more meaningful comparison; here, again, the agreement is good. On the other hand,

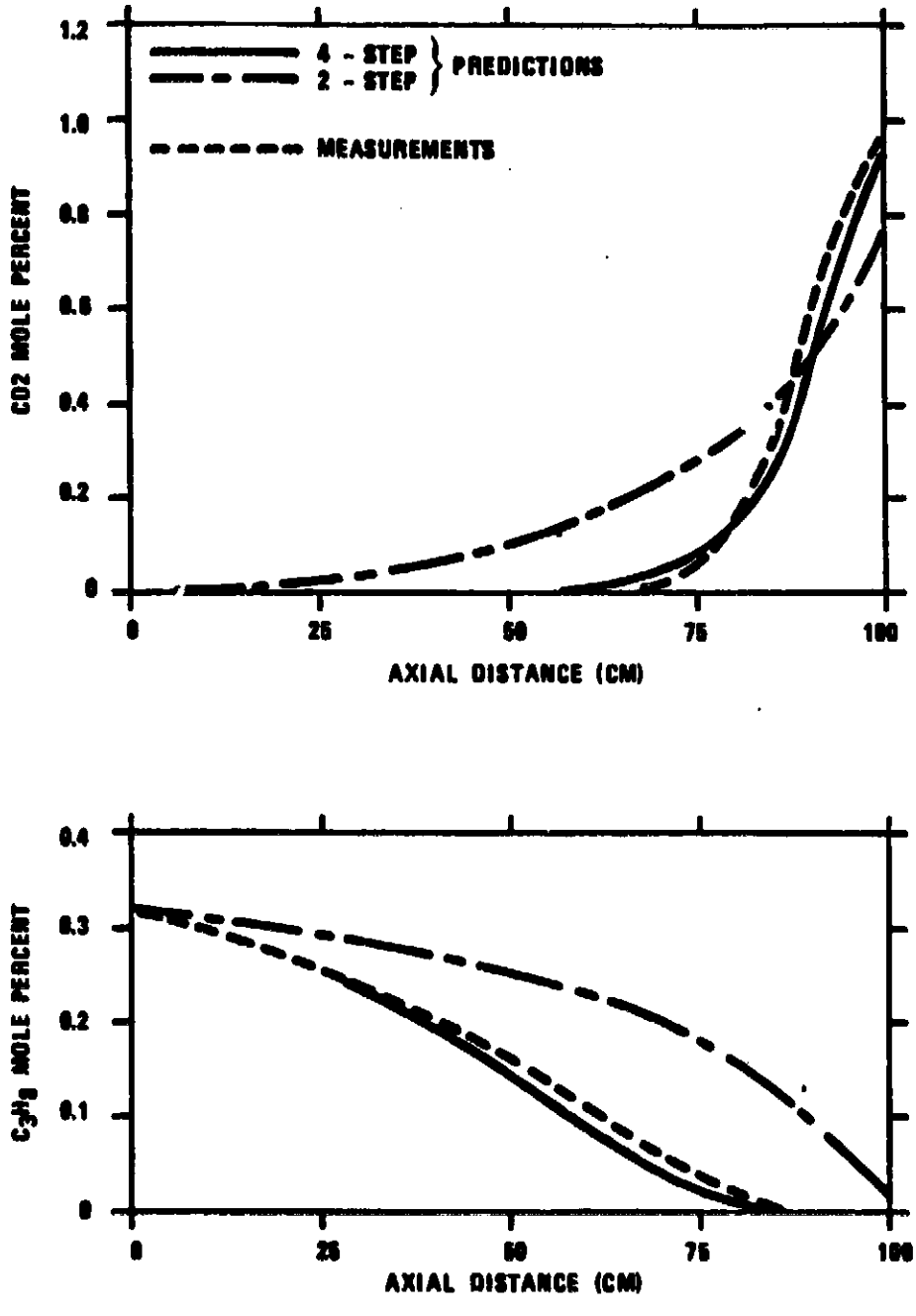


Figure 1a. Lean C_3H_8 Flame ($\phi = 0.12$).

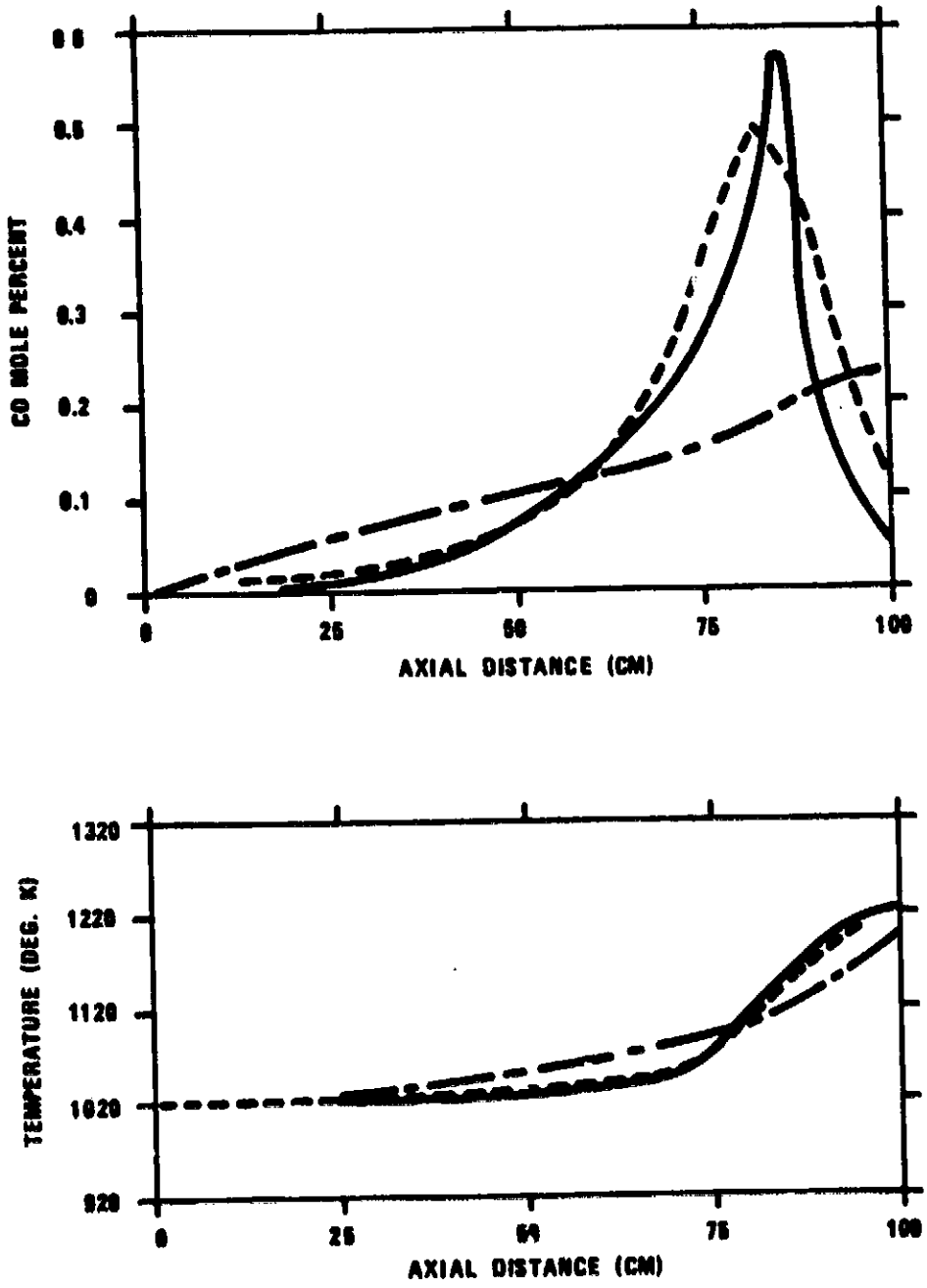


Figure 1b. Lean C_3H_8 Flame ($\Phi = 0.12$).

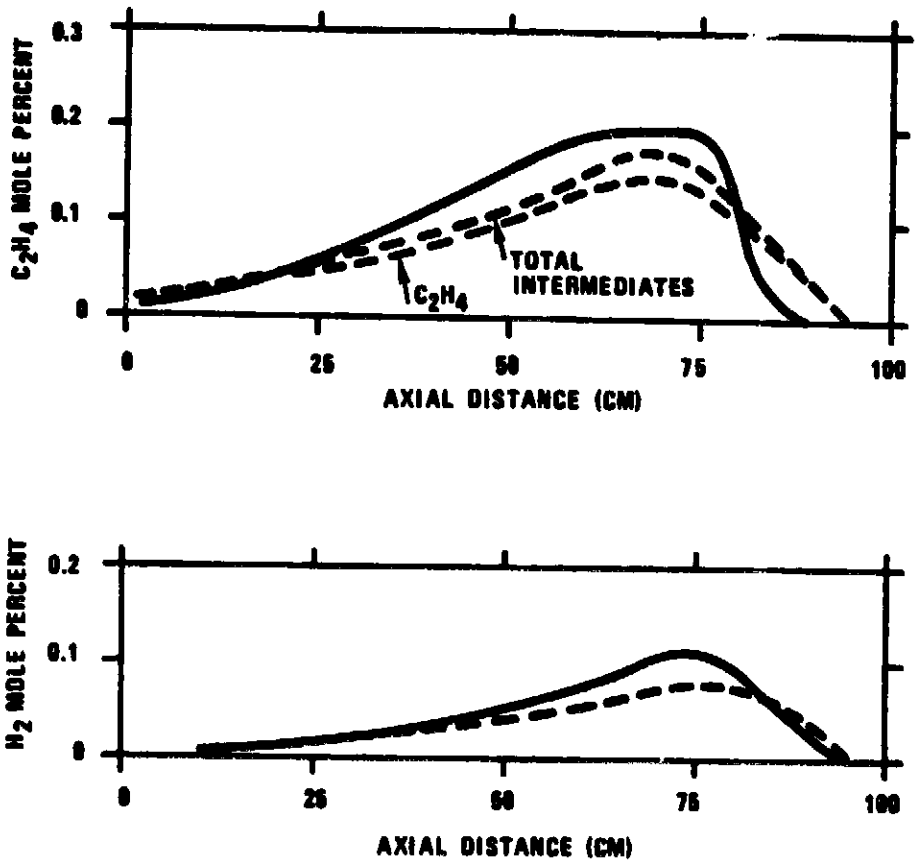


Figure 1c. Lean C_3H_8 Flame (ϕ = 0.12).

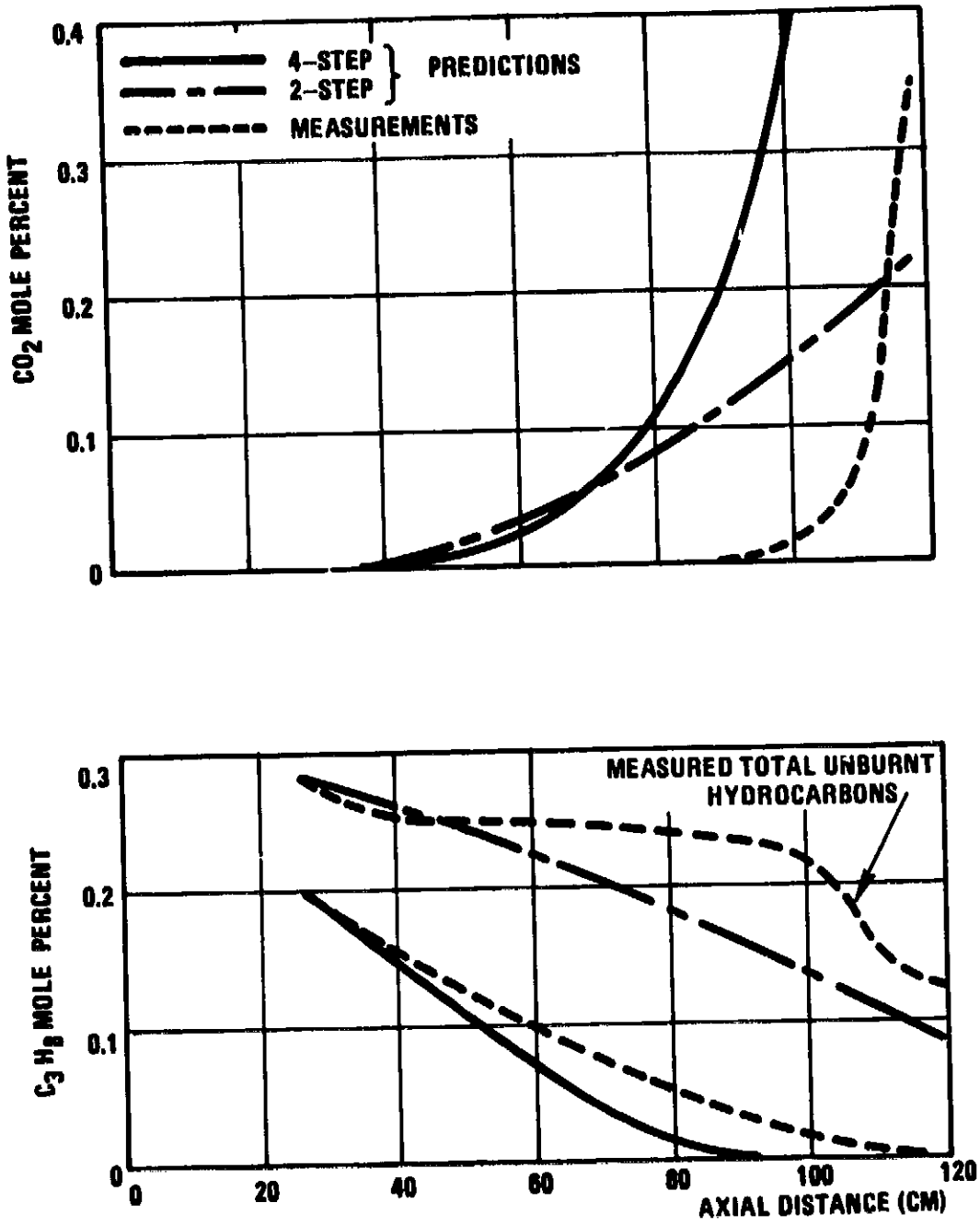


Figure 2a. Stoichiometric C_3H_8 Flame (ϕ=0.98).

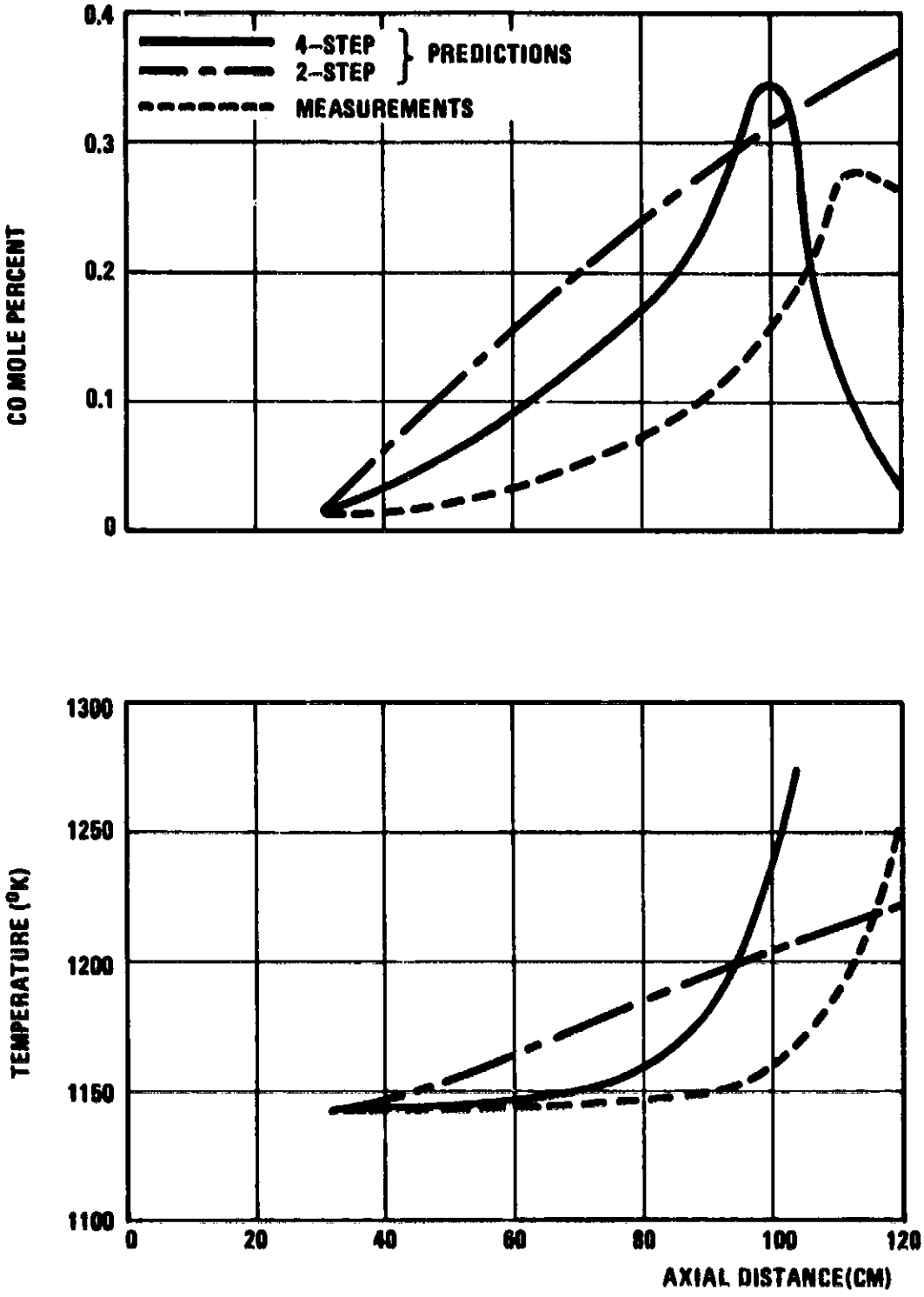


Figure 2b. Stoichiometric C_3H_8 Flame (ϕ=0.98).

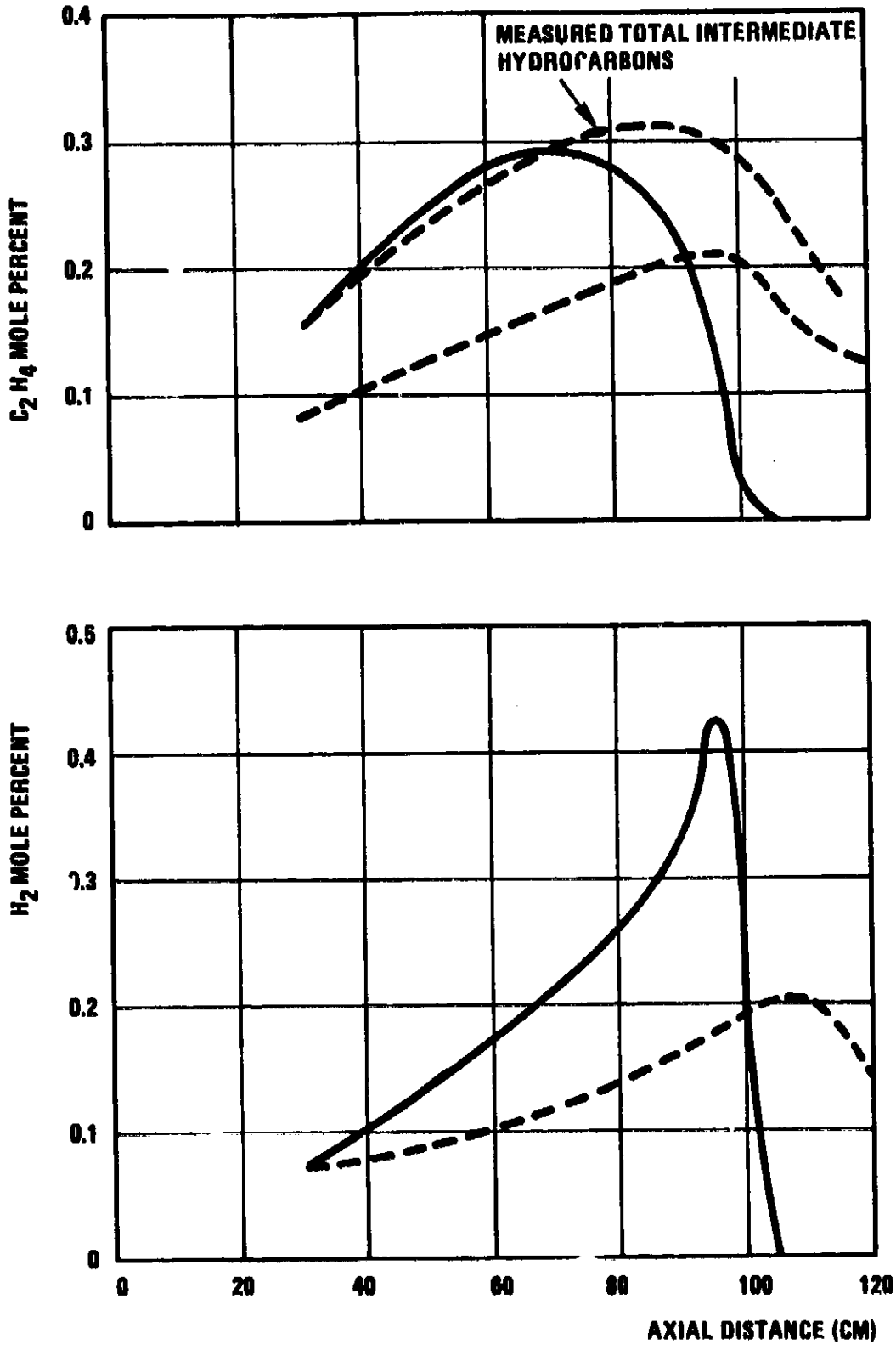


Figure 2c. Stoichiometric C_3H_8 Flame (ϕ=0.98).

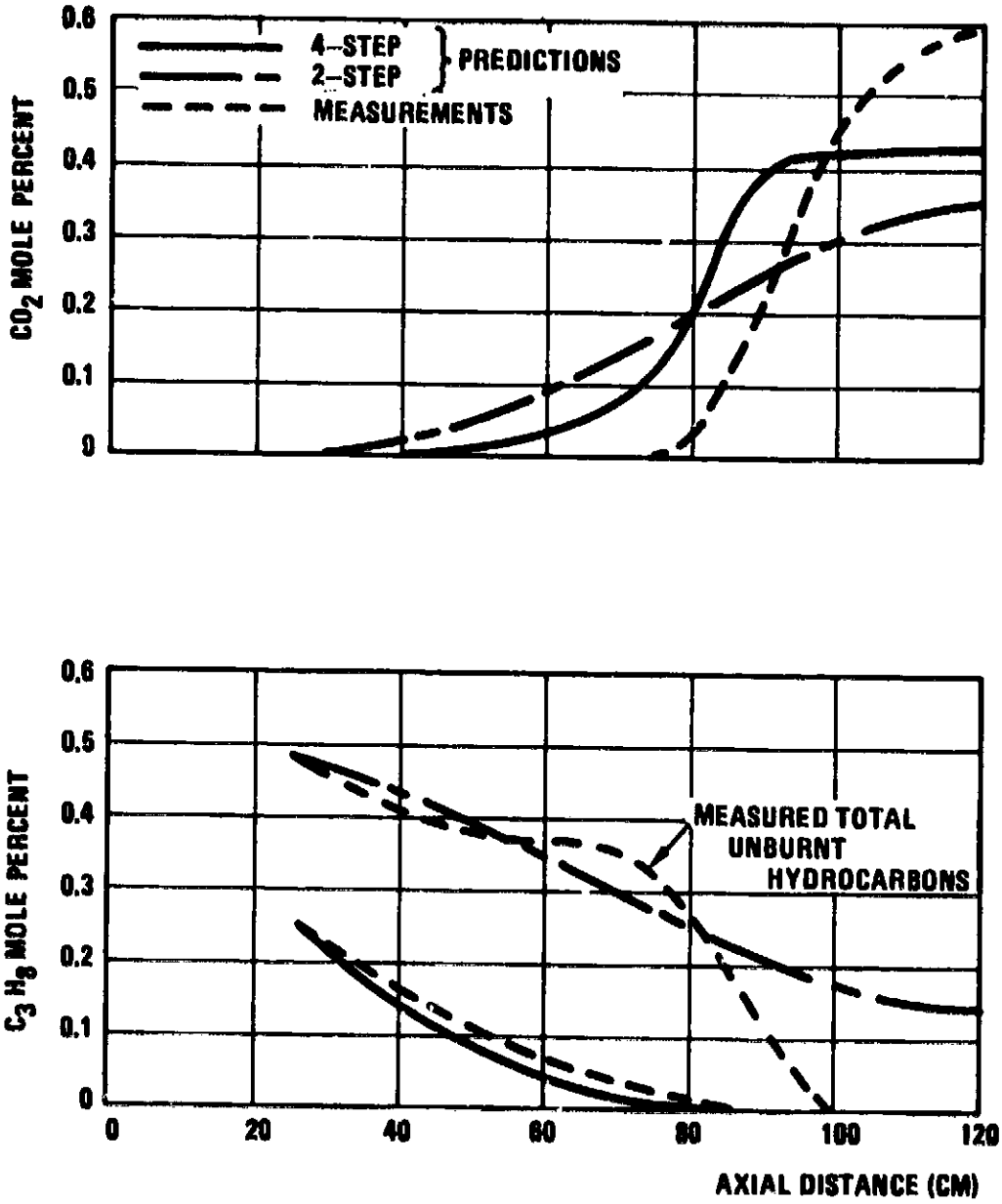


Figure 3a. Rich C_3H_8 Flame (ϕ=1.59).

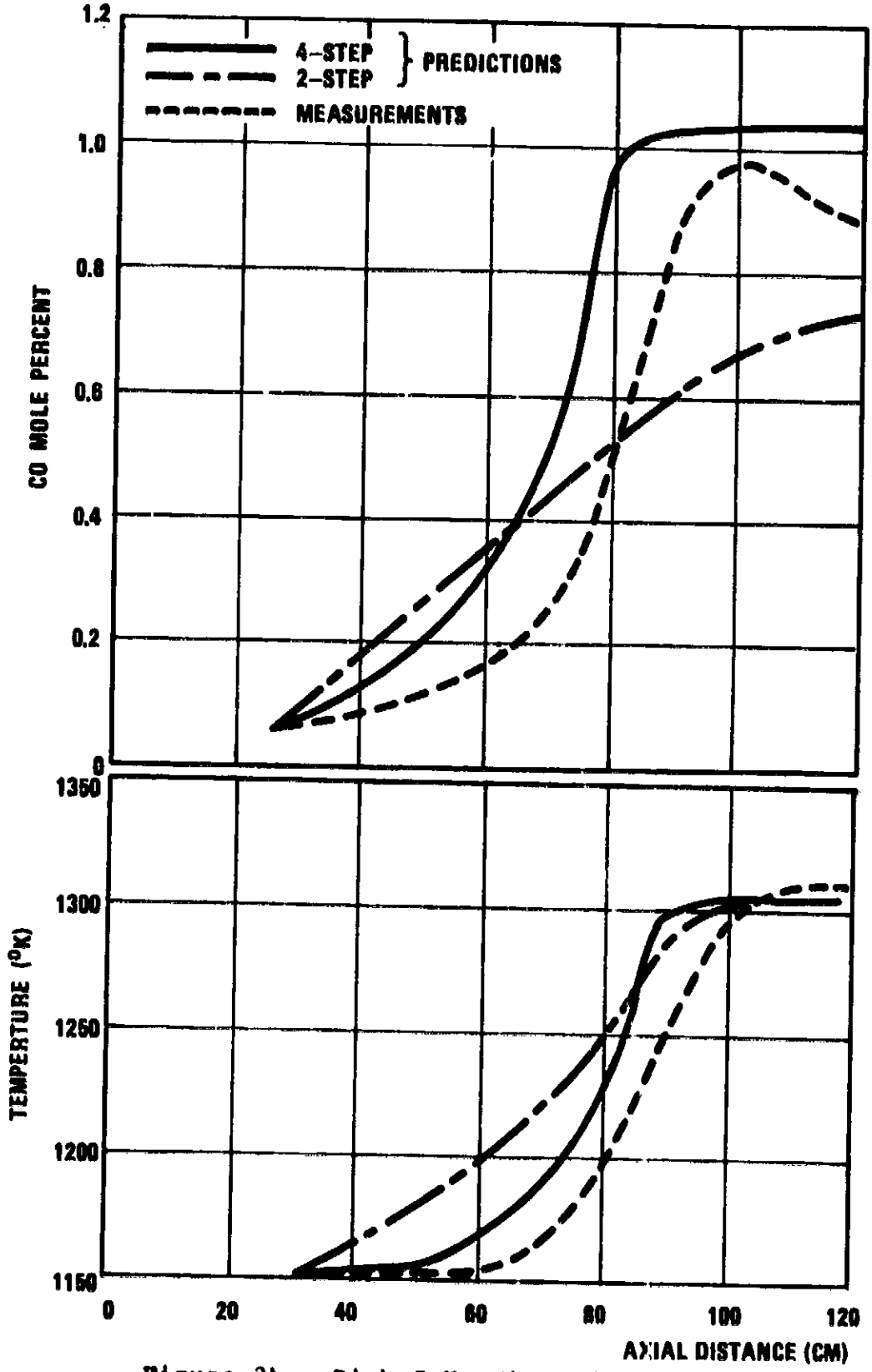


Figure 3b. Rich C_3H_8 Flame (ϕ=1.59).

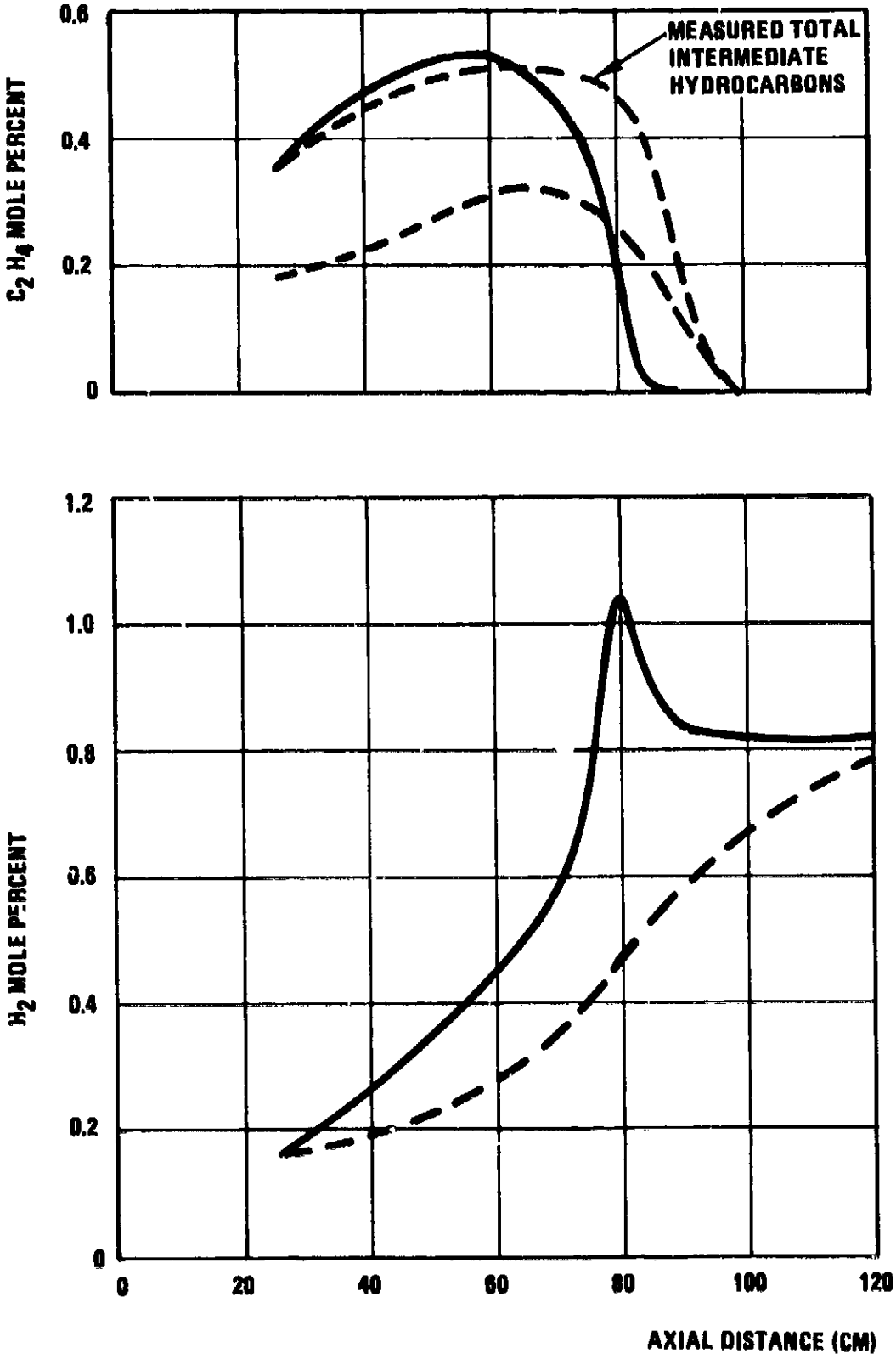


Figure 3c. Rich C_3H_8 Flame (ϕ=1.59).

the two-step predictions show considerable discrepancy for all the species and for the temperature.

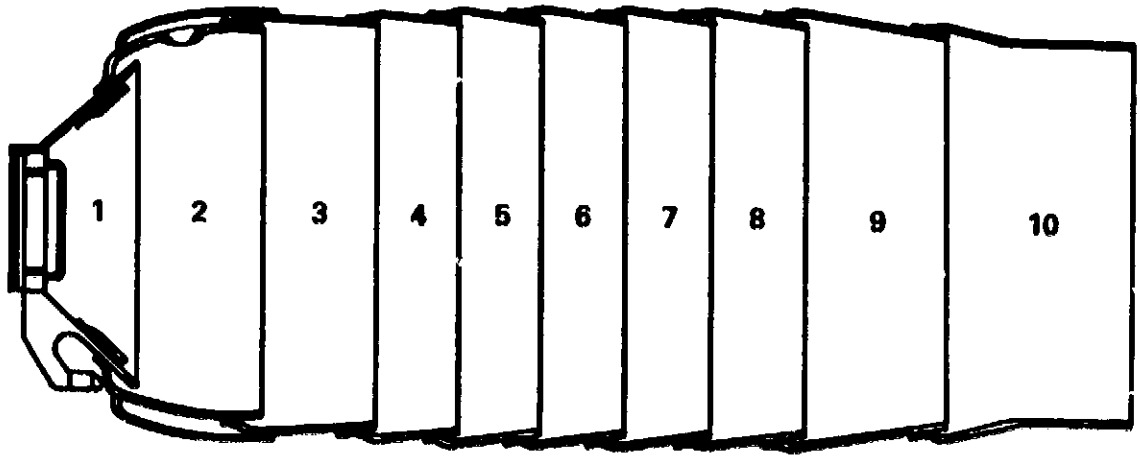
Figure 2 (a, b, and c) shows the measurements and predictions for the stoichiometric case. Here the four-step predictions are not as good as for the lean case; however, compared to the two-step predictions, the four-step results are in much closer agreement with the measurements. A major discrepancy is the predicted (four-step) H_2 concentration, which is considerably higher than the measured values.

Figure 3 (a, b, and c) shows the measurements and predictions for the fuel-rich case. Here, again, the four-step predictions, although not in very close agreement with the measurements, are far superior to the two-step predictions. The four-step fuel concentration and temperature profiles are in good agreement with the measurements; CO, CO_2, and C_2H_4 are in fair agreement. Again, the H_2 concentration is overpredicted as in the stoichiometric case.

As shown by these results, a problem not resolved with the four-step scheme is the discrepancy between predicted and measured H_2 and H_2O concentrations, especially at stoichiometric and fuel rich conditions. The H_2 oxidation rate is predicted to occur more slowly, and results in an excess of H_2 and under-prediction of H_2O, as compared to the measurements. A similar observation was also made by Hautman, et al.[53]

B. JT8D Combustor Computations

The 3-D Combustor Performance Program was set up and run for a JT8D-17 combustor as shown in Figure 4. This combustor uses a single pressure atomizing injector on the centerline of the can. Air is admitted around the injector through a 45-degree swirler. The operating points for the computations represent idle, cruise, and take-off and are given below:



FUEL INJECTOR AND PRIMARY SWIRLER EQUIVALENT METERING AREA 7.61 PERCENT

Equivalent Metering Area

Louver Cooling Air		Combustion Air	
Panel	%	Panel	%
1	1.53	2	7.93
2	5.62	3	1.92
3	7.56	5	8.00
4	5.69	8	15.85
5	4.24	9	18.09
6	3.41		
7	3.42		
8	3.43		
9	2.78		
10	1.81		

Figure 4. JT8D-17 Combustor.

Condition	Airflow lbs/sec	Pressure psia	Temperature °F	Fuel/Air Ratio
Idle	4.06	39.6	260	0.0074
Cruise	7.87	103.0	657	0.0138
Take-Off	16.45	256.0	825	0.0182

The steps adopted in the solution procedure for the JT8D combustor are outlined below:

(1) The 3-D combustor program was used to solve for the variables: velocity, pressure, turbulence energy and dissipation, enthalpy (temperature), mixture fraction, mass fractions of unburned fuel, C_xH_{y-2}, CO, and H_2. At this stage, the soot and radiation equations were not solved, and the solution was carried on until a convergence level of approximately 5 percent in cumulative mass residual was reached.

(2) The soot and radiation equations were solved next. The radiation fluxes appear as sources in the enthalpy equation; and this, in turn, influences the other dependent variables. The solution of the variables in Step (1) was repeated coupled with the soot and radiation equations. The process was continued until a convergence level of approximately 1 percent was reached.

(3) The NO_x equations were solved next. The solution of the variables in Steps (1) and (2) was repeated, coupled with the NO_x equations. The process was continued until the convergence level desired for the final solution (~0.5 percent) was reached.

The reason for adopting the above stepwise procedure was to cut down on required computer time. Since the soot is generally present only in small concentrations, it will influence the main flow field only slightly and so delaying the solution of the soot and radiation (which is mainly from soot) equations resulted in a considerable saving of computer time. Similarly, the NO_x species have an even smaller influence on the other variables and so their solution was further delayed. Due to the point-by-point nature of the NO_x solution, this solution had to be repeated a number of times to achieve convergence, as explained in Chapter V.

A flow chart of the overall solution procedure is given in Figure 5. The various steps are executed automatically by the program from start to completion.

Computations were performed with both the two-step and four-step hydrocarbon oxidation schemes and with a grid of 10 x 10 x 5 (axial x radial x tangential) points. Due to the coarseness of the grid, it was not possible to simulate exactly all of the geometrical details of the combustor. However, the main features were simulated as closely as possible. Due to the large computer times required for the NO_x calculations, as explained in Chapter V, increasing the number of grid points significantly over that used was found to be computationally prohibitive.

The central processor time on a CYBER 730 computer with the two-step hydrocarbon scheme was 0.044 seconds per iteration per internal node (boundary nodes that are not calculated are excluded here) when the NO_x chemical kinetics solution was not activated. For the NO_x solution, the central processor time was an additional 0.2-0.3 second per iteration per internal node. Typically 100-150 iterations were required before the NO_x solution was turned on, after which an additional 50-100 iterations were required to achieve convergence. Thus for the chosen grid (10 x 10 x 5), a complete run required 3000-5000 seconds depending on the conditions

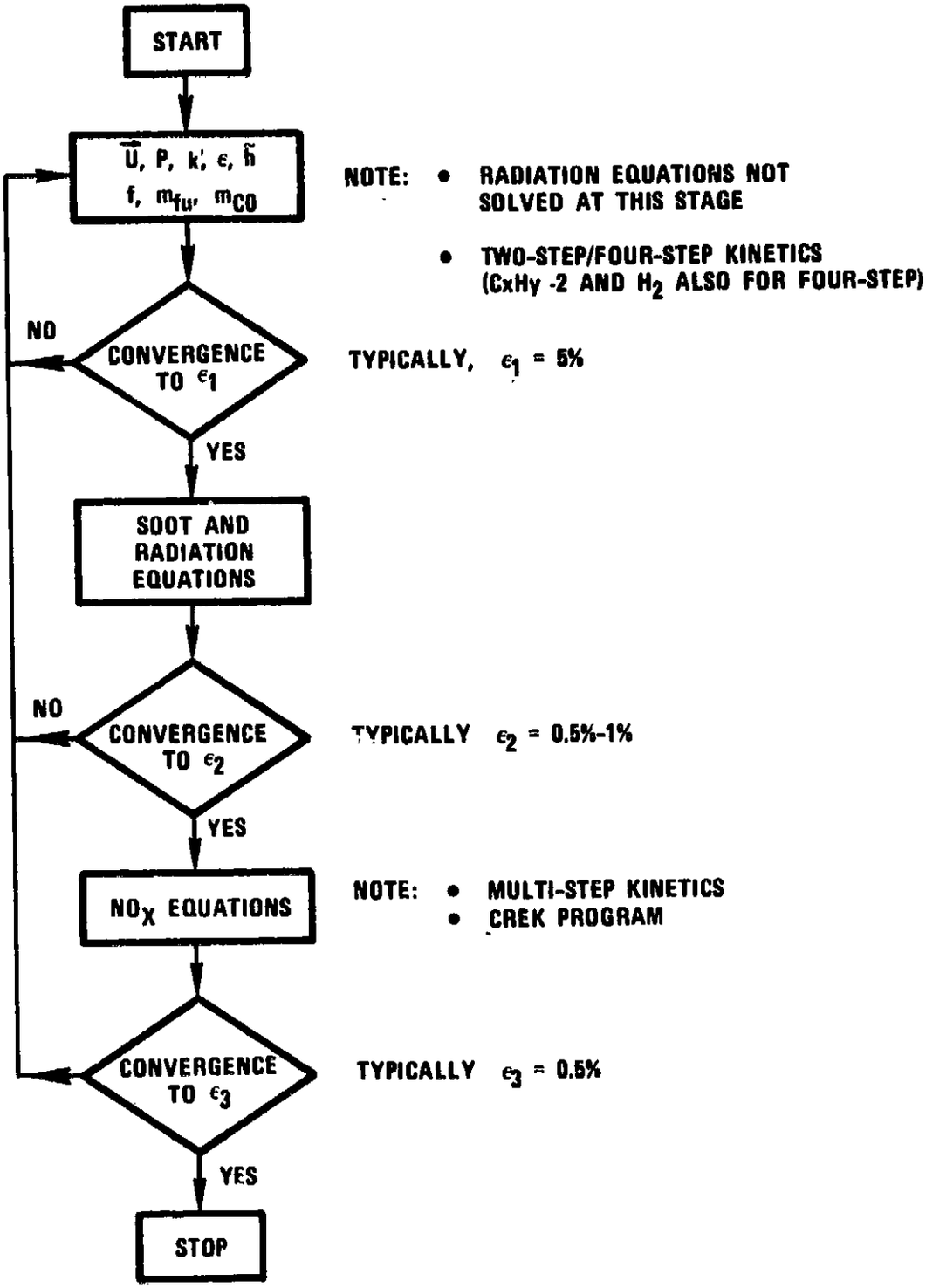


Figure 5. Flowchart of Overall Solution Procedure.

for the run (which influences the number of iterations to convergence), with the bulk of the time spent on NO_x calculations. Since the four-step scheme involved the solution of additional equations for the intermediate hydrocarbon and H_2, the computation times were about 10-15 percent higher than those with the two-step scheme. The central memory required for the 10 x 10 x 5 grid was 173,500 octal words.

The predicted emissions index for the idle, cruise, and takeoff conditions with the two-step and four-step schemes is shown in Tables IIa and IIb. For the idle case, the predicted smoke concentration is very small and much lower than that experimentally observed. The formation of soot, as modeled, is governed by the local temperature and fuel/air ratio and also turbulent fluctuations. Since the temperature and fuel/air ratio are low for the idle case, the model does not predict significant soot formation. Obviously, other factors that have not been modeled and that are not precisely known, govern soot formation under such conditions.

For the cruise and takeoff cases, the emissions indices for soot and NO_x show the correct trends and are reasonably close to the measurements that are available. The differences between the two-step and four-step schemes are not significant in the prediction of the emissions index, which represents an integrated value at the combustor exit. The differences in the two schemes are significant in the primary zone of the combustor.

The predicted radiation flux to the combustor wall for the conditions of idle, cruise, and takeoff is shown in Table IIIa for the two-step scheme and in Table IIIb for the four-step scheme. The values are reported at the primary, secondary, and tertiary zones which are at 6, 21, and 33cm downstream of the fuel nozzle; these correspond to the locations at which measurements were conducted by Claus[56] for different operating conditions. The predicted radiation fluxes show the correct trends; i.e., the flux is

TABLE IIa. PREDICTED EMISSIONS INDEX WITH TWO-STEP HYDROCARBON OXIDATION SCHEME.

Condition	Emission Index Gm of Emissions/Kg of Fuel	
	Smoke	NO_x
Idle	0.26 E-3 (0.6)[55]	≈0
Cruise	1.6	15
Takeoff	1.5 (2.8)[55]	28 (24.4)[54]

NOTE: Values in parentheses are experimental measurements from indicated reference.

TABLE IIb. PREDICTED EMISSIONS INDEX WITH FOUR-STEP HYDROCARBON OXIDATION SCHEME.

Condition	Emission Index Gm of Emissions/Kg of Fuel	
	Smoke	NO_x
Idle	0.056 (0.6)[55]	≈0
Cruise	1.3	13
Takeoff	1.2 (2.8)[55]	27 (24.4)[54]

NOTE: Values in parentheses are experimental measurements from indicated reference.

TABLE IIIa. PREDICTED WALL RADIATION FLUX WITH TWO-STEP HYDROCARBON OXIDATION SCHEME.

Condition	Primary Zone (W/M^2)	Secondary Zone (W/M^2)	Tertiary Zone (W/M^2)
Idle	2.9E4	3.46E4	1.03E4
Cruise	5.55E5	8.98E5	2.23E5
Takeoff	7.89E5	1.33E6	4.26E5

TABLE IIIb. PREDICTED WALL RADIATION FLUX WITH FOUR-STEP HYDROCARBON OXIDATION SCHEME.

Condition	Primary Zone (W/M^2)	Secondary Zone (W/M^2)	Tertiary Zone (W/M^2)
Idle	1.06E4	1.35E4	3.19E3
Cruise	3.78E5	9.01E5	2.13E5
Takeoff	6.40E5	1.34E6	3.72E5

maximum in the secondary zone and minimum in the tertiary zone. This trend was experimentally observed by Claus.[56] The level of the flux also corresponds to that measured by Claus for slightly different conditions. Due to the differences in the conditions for which measurements and predictions were made, a direct comparison of the two is not shown.

For the idle case, since the soot concentrations were predicted to be very low, the predicted radiation fluxes are also towards the low side. The predicted radiation flux with the four-step scheme is lower than that with the two-step scheme for the idle case, but the soot predictions show the opposite trend, i.e., slightly higher with the four-step scheme. This occurs because, in the predictions for the idle case, the radiation from the soot is low and is due to its small concentration. The gas radiation is important and is predicted to be higher with the two-step scheme because of a faster temperature rise.

The computations performed for the three operating conditions of the JT8D combustor show that the present model is capable of producing reasonable predictions of the emissions of smoke and NO_x and of the wall radiation flux.

CHAPTER VIII

CONCLUSIONS

In the present work, a method was formulated for the following:

- computation of soot and NO_x emissions from a combustor
- inclusion of the effects of soot on radiant heat transfer, and
- extension of the two-step hydrocarbon oxidation scheme to a four-step one.

The method was coded into the Garrett 3-D Combustor Performance Program. A description of the program, list of Fortran variables, and program listing have been included in the report to aid the reader in understanding the emissions model.

The computations that were performed show that the method is capable of producing reasonable results. The lack of accurate experimental data has precluded more detailed validation of the model. As reliable experimental data becomes available, further computations will reveal the capabilities and limitations of the model and the modifications necessary to overcome the limitations.

CHAPTER IX

NOMENCLATURE

All symbols were defined in the report at the point when first referenced. The following is a list of symbols used often in the report.

a = Absorption coefficient

C_i = Time-mean concentration of species i

C_p = Specific heat

D = Particle diameter

E = Activation energy

k = Kinetic energy of turbulence

K_b = Backward reaction rate constant

K_C = Equilibrium constant

K_f = Forward reaction rate constant

m_i = Mass fraction of species i

n = Nuclei concentration

n_o = Rate of spontaneous nuclei formation

N = Concentration of soot particles

P = Pressure

R = Reaction rate

S = Scattering coefficient

S_ϕ = Source term of dependent variable ϕ

t = Time

T = Temperature

$\vec{u}$ = Velocity vector

ϵ = Emissivity; dissipation rate of turbulence

ϕ = General dependent variable

ν = Kinematic viscosity

μ_t = Effective viscosity

σ = Stefan-Boltzmann constant

σ_ϕ = Prandtl/Schmidt number of dependent variable ϕ

ρ = Density

λ = Wavelength

Subscripts

fu = Fuel

i = Species i

n = Nuclei

O_2 = Oxygen

pr = Products

S = Soot

ϕ = Dependent variable

Superscripts

* = Fine structure

° = Surrounding fluid

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APPENDIX A

DESCRIPTION OF THE 3-D COMBUSTOR PERFORMANCE PROGRAM

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DESCRIPTION OF THE 3-D COMBUSTOR PERFORMANCE PROGRAM

The 3-D performance model is a three-dimensional recirculating-flow program that is capable of analyzing a variety of combustor configurations, including can, can-annular, and annular. The program solves for the three velocity components, U, V, and W, species concentrations, C_XH_Y, C_XH_{Y-2}, C(S), CO, CO_2, H, H_2, O, O_2, OH, H_2O, N, N_2, NO, NO_2, turbulence quantities from the k-ϵ turbulence model, and three radiation fluxes. In addition, the use of primitive variables makes modifications to the boundary conditions easy, allowing the user to analyze complex inlet geometries. Also provided is a subroutine for calculating the trajectories and evaporation rates of a fuel-nozzle spray. The functions of the various subroutines are briefly described below.

Program MAIN (a computer listing has been provided in Appendix D) is divided into two basic sections. Up to card MA.167, the routine is concerned with reading the input data and converting it to the program's internal units which are Systeme International (S.I.). The input sequence is covered in Appendix B so only the units will be discussed. Cards MA.7 to MA.11 are used to define seven arrays which convert lengths associated with dimensions and lengths associated with velocity, energy, mass, temperature, pressure, and angles respectively. By proper specification in the data statements, the user may employ those input units that are most convenient. The output units are always S.I. From card MA.168 on, MAIN's function is to call the other various routines in their proper sequence.

Subroutine INIT performs some preliminary calculations (AL.10 to AL.155), prints the input data (AL.156 to AL.258), and defines

the initial conditions and some of the boundary conditions on the various arrays (AL.259 on). In section AL.48 through AL.78, two arrays, JKIN and IKIN, are defined. They merely contain flags which indicate the locations of mass injection points. Cards AL.261 to AL.272 contain logic for the restart option. If Tape 8 from a previous run is saved and then made available for use during a subsequent run, the program will read the initial and boundary conditions from it.

Subroutine ALLMOD contains several entry points which perform miscellaneous calculations pertaining, usually, to the boundary nodes where modifications to the standard equation are in order. The cyclic nature of the boundary conditions in the θ or K direction is evident in FMOD as well as limits to the species mass fractions. VELMOD allows the inlet swirl velocity to be increased gradually over a number of iterations and assures that overall continuity is maintained at the exit plane. DENMOD makes alterations to the density at the boundaries to maintain the correct mass-flow rate. GAMOD specifies the wall viscosity values as calculated by the wall functions. SOMAS is used to initialize an array DIVG which is used later in the program. The largest entry point SOMOD contains logic for modifying the equation coefficients and source terms when cooling slots, walls, and droplet evaporation are present. Each variable has its own section and accounts for transfer with the walls and mass addition from the evaporating fuel. SOMODZ deals only with the Z-direction radiation equation and is in a section alone as the data storage is slightly different for this variable.

Subroutine OUTPUT is used for printout purposes. The emissions index of SOOT and NO_x is calculated and printed here. Subsequently, subroutine FPRINT is called for the printout of all dependent variables.

Subroutine AUX performs the auxiliary calculations for temperature, density, viscosity, and source terms. Entry DENS uses AU.11 to AU.56 to calculate temperature. Cards AU.52 to AU.56 limit the values calculated in order to account for dissociation and early iteration fluctuations. With known temperature, density is then determined from AU.57 to AU.108. VISCO obtains effective viscosity from turbulent kinetic energy and dissipation and calculates Y+ for use by the wall function routine. GAMMA obtains the effective diffusion coefficients. SOURCE contains all calculations for source terms with the exception of the aforementioned modifications in SOMOD. Again, each variable has its own section, with coding that is quite straightforward and requires no explanation.

Subroutine AUXRAD performs the same function as AUX except that it pertains only to the radiation equations.

Subroutine SPRAY is used to determine the evaporation rate of the fuel-nozzle spray. A large section, from SP.106 to SP.269, deals with locating the droplet, determining free-stream conditions, and handling the situation where the droplet approaches a boundary. Next, various fuel and free-stream properties are evaluated (to SP.292). The drag forces and time step are then determined and used to obtain new velocities and location. If the droplet is below the boiling temperature, no evaporation occurs (SP.340 to SP.347); but, when the boiling temperature is reached, evaporation rates are calculated, and the appropriate entries to the evaporation array (EVAP) are made. Information concerning momentum changes due to evaporation are also stored in their respective arrays and later (SP.382 to SP.425) on a scratch file for use when the three momentum equations are solved.

The coefficients for each variable are generated and the solution routine called in subroutine STRIDE. First, equations for U,

V, and W are handled (ST.117 to ST.632), then the pressure perturbation (P') is obtained (ST.633 to ST.714) and used to correct the velocities (ST.716 to ST.753) so that mass errors are reduced. Then, the remaining variables are solved with the radiation equations having their own special section (ST.915 to ST.937). The chemical kinetics calculations are contained from NOX.230 to NOX.342. Here the inputs to program CREK are prepared and the outputs from CREK are stored in the respective arrays.

STRAD is a subroutine used in the radiation model which performs the same function as STRIDE performed for the other variables.

Subroutines ABSORB, ASYMP, CHEBY, DLECK, EGAS, PENTA, SOOT and SCRTCH (from Ref. 40) are used to compute the absorbtivity of gas-soot mixtures.

SOLVE provides a solution to the equations generated in STRIDE. A full three-dimensional solution would be time consuming and would require enormous computer storage. Therefore, an approximate solution is obtained by "sweeping" through the field several times alternately solving along one direction, while holding the values in the other two fixed. The variable ICTDMA (NV) at S0.36 is used to specify the number of such sweeps. As the program converges, and the variables assume their final values, the solution becomes more accurate. Due to the cyclic nature of the boundary conditions in the θ-direction, a cyclic tri-diagonal matrix algorithm (CTDMA) is used for this direction; the coding sequence is contained in SOLVE2.

Subroutine FPRINT is used for the printout of field values of dependent variables.

The last part of the program contains the chemical kinetics subroutines: CREK, CALC, SPECE, CREKO AND HCPS.

Subroutine CREK is the main routine called from the 3-D program. It controls the solution strategy: equilibrium or kinetic and problems associated with lack of convergence.

Subroutine CALC construct the Newton-Raphson correction matrix for both equilibrium and kinetic states and solves for the corrections by a standard Gaussian elimination procedure. In the present work, modifications have been made to this subroutine in order to incorporate the four-step hydrocarbon oxidation scheme and to compute the reaction rates from the eddy-break-up model.

Subroutine SPECE contains the Newton-Raphson iteration procedure for both equilibrium and kinetic states.

Subroutine CREKO is the initializing subroutine and is used for the input of element, thermodynamic and reaction mechanism data.

Subroutine HCPS is used for computing the enthalpy, constant pressure specific heat and the entropy of the species.

Further details of the chemical kinetics subroutines are contained in Ref. 48.

APPENDIX B

PROGRAM INPUT

DESCRIPTION

APPENDIX B

PROGRAM INPUT DESCRIPTION

Card Set	Variable	Format	Description
1	TITLE	20A4	Each card is a heading for a particular three-dimensional array that is printed out. These never change (33 cards).
2	TITLE2	10A4	Case title card.
3	LP1	8(I2,8X)	Number of grid nodes in axial (x) direction.
	MP1		Number of grid nodes in radial (y) direction.
	NP1		Number of grid nodes in tangential (z) direction.
	IPLAX		01 For plane geometry; 02 For axisymmetric geometry.
	MODEL		01 For laminar viscosity; 02 For k-ϵ viscosity model.
	MODER		01 For kinetic controlled combustion; 02 for kinetic and turbulence controlled combustion.
	IPAR		01 For absolute pressure; 02 For relative pressure.
	ITRAD		01 No radiation; 02 With radiation; radiation properties specified; 03 With radiation; radiation properties calculated.
4	IU	8(I2,8X)	01 Input units are international system (i.e., meters, kilograms, degrees kelvin, newtons, joules, radians, seconds or combinations thereof); 02 User selected input units.
	MODEN		01 Density is fixed at the value of "Den" on Card Set 19; 02 Density calculated from perfect gas law.
	INTAPE		00 Initial conditions not printed; 08 Initial conditions printed.

Card Set	Variable	Format	Description
	IDW		00 Inner boundary is axis of symmetry; 01 Inner boundary is wall.
	IRES		00 This is a new case; 01 This is a restart of previous case.
5	ISOLVE	8(I2,8X)	An 01 in proper field indicates that this particular variable will be solved for; an 00 indicates that it will not be. Order of variables: u, v, w, p', k, ϵ, ϕ, m_{fu}, m_{CH}. m_{CO}, m_{H_2}, $\tilde{h}$ n, s1, s2, 14*0 (14 species solved by CREK), Rx, Ry, Rz.
6	ICTDMA	8(I2,8X)	Indicates the number of "sweeps" made in the solve routine for each variable. Order of variables as in Card Set 5.
7	IPRINT	8(I2,8X)	An 01 indicates that this variable will be printed, an 00 indicates that it will not be. Order of variables as in Card Set 1.
8	RELAX	8E10.4	Relaxation parameters for each variable. Order of variables as in Card Set 5. In addition, pressure, density, effective viscosity at end of the set.
9	PR	8E10.4	Laminar Prandtl numbers for each variable. Order of variables as in Card Set 5.
10	PREF	8E10.4	Turbulent Prandtl numbers for each variable. Order of variables as in Card Set 5.
11	X	8E10.4	X-coordinates (LP1 values).
12	RI	8E10.4	Radius of inner boundary.
	Y		Y-coordinates as measured from inner boundary (MP1-1) values. Since Y(1) is <u>always</u> 00, RI is read in its place.
13	Z	8E10.4	Z-coordinates (NP1 values).
14	IWEI	8(I2,8X)	I-node at which upstream inclined wall ends.
	JWIO	See Fig. B-1	J-node at which upstream outer inclined wall starts.

Card Set	Variable	Format	Description
	IWEO		I-node at which downstream inclined wall starts.
	JWOO		J-node at which downstream outer inclined wall ends.
15	IWLI	8(I2,8X)	Starting I-nodes of the calculation domain when inclined wall is present. (Skip if IWEI = 2).
16	JWLO	8(I2,8X)	Ending J-nodes of the calculation domain at upstream outer inclined wall. (Skip if IWEI = 2).
17	IWLO	8(I2,8X)	Ending I-nodes of the calculation domain when inclined wall is present. (Skip if IWEO = L).
18	JWLO	8(I2,8X)	Ending J-nodes of the calculation domain at downstream outer inclined wall. (Skip if IWEO = L).
19	PRESS	8E10.4	System pressure.
	DEN		The value of density if option MODEN = 01 is selected.
	ABSOR		Absorption coefficient in radiation model (if ITRAD = 2).
	SCATR		Scattering coefficient in radiation model (if ITRAD = 2).
	AKFAC		Internally defined turbulent kinetic energies are AKFAC time the appropriate velocity squared.
	ALFAC		Internally defined turbulent length scales are ALFAC time the appropriate distance.
20	CXX	8E10.4	Carbon atoms in fuel modecule.
	HYY		Hydrogen atoms in fuel molecule.
	HFU		Heat of formation of fuel.
	FUMCO		Initial value assigned to M_{CO}.
21	PREXP1	8E10.4	Preexponent of 1st reaction.
	ARCON1		Activation energy divided by gas constant of 1st reaction (E/R).
	CR1		Constant in turbulence controlled reaction rate of 1st reaction.

Card Set	Variable	Format	Description
	PREXP2		Pre-exponent of 2nd reaction.
	ARCON2		Activation energy divided by gas constant of 2nd reaction (E/R).
	CR2		Constant in turbulence controlled reaction rate for 2nd reaction.
22	PREXP3	8E10.4	Pre-exponent of 3rd reaction.
	ARCON3		Activation energy divided by gas constant of 3rd reaction (E/R).
	CR3		Constant in turbulence controlled reaction rate for 3rd reaction.
	PREXP4		Pre-exponent of 4th reaction.
	ARCON4		Activation energy divided by gas constant of 4th reaction (E/R)
	CR4		Constant in turbulence controlled reaction rate for 4th reaction
23	AA1	8E10.4	Exponent on species concentration
	BB1		in the reaction rate for 1st
	CC1		reaction.
	AA2		Exponent on species concentration
	BB2		in the reaction rate for 2nd
	CC2		reaction.
24	AA3	8E10.4	Exponent on species concentration
	BB3		in the reaction rate for 3rd
	CC3		reaction.
	AA4		Exponent on species concentration
	BB4		in the reaction rate for 4th
	CC4		reaction.
25	C1	8E10.4	Turbulence model constant.
	C2		Turbulence model constant.
	CD		Turbulence model constant.
	AMU		The value of the viscosity if option MODEL = 01 is specified. Also the laminar viscosity used in the "wall functions".
	ERROR		Program will terminate if total error in mass becomes less than this value.
	TCYLW		Temperature of cylindrical portion of combustor and of dome.
	TLIP		Temperature of cooling slot lip.
26	LASTEP	2(I3,7X),	Maximum number of iterations.
	IJUMP	6(I2,8X)	Number of iterations between array printout.

Card Set	Variable	Format	Description
	JSW1		J-node at start of dome inlet.
	JSW2		J-node at end of dome inlet.
	NUINJ		Number of axial injection points (cooling slots).
	NVINJ		Number of radial injection points.
27	USW	8E10.4	Axial velocity of dome inlet.
	VSW		Radial velocity of dome inlet.
	SWNO		Ratio of tangential to axial velocity at dome inlet.
	AFSW		Flow rate of fuel and air through dome inlet.
	FSW		Flow rate of fuel through dome inlet.
	TSW		Temperature at dome inlet.
28	NFNZ	2(I2,8X), 6E10.4	00 No liquid fuel nozzle; 01 Liquid fuel nozzle present.
	ISPRAY		Droplet evaporation routine is called. every ISPRAY iterations.
	TFUEL		Initial temperature of liquid fuel.
29	XO	8E10.4	X-location of origin of fuel nozzle spray.
	YO		Y-location of origin of fuel nozzle spray.
	ZO		Z-location of origin of fuel nozzle spray
	ALFA		Nozzle cone angle.
	BETA		Nozzle back angle.
	DELTA		Nozzle down angle.
	THETA1		Initial spray cone segment angle.
	THETA2		Final spray cone segment angle.
	RNSL		Number of spray cone rays.
	WFF		Fuel flow rate.
	SMD		Sauter mean diameter.
	VFUEL		Initial fuel droplet velocity.
	RFUEL		Radius of fuel nozzle. (Skip Set 29 if NFNZ=0)
			Skip Sets 30-35, if NUINJ=0.
30	IUINJ	8(I2,8X)	I node location of cooling slots
31	JUINJ	8(I2,8X)	J node location of cooling slots.
32	UINJ	8E10.4	Cooling slot axial velocity.
33	WUINJ	8E10.4	Cooling slot tangential velocity.

Card Set	Variable	Format	Description
34	AUINJ	8E10.4	Cooling slot mass flow rate.
35	TUINJ	8E10.4	Cooling slot temperature.
			Skip Sets 36-43, if NVINJ=0.
36	IVINJ	8(I2,8X)	I node location of radial injection.
37	JVINJ	8(I2,8X)	J node location of radial injection
38	KVINJ	8(I2,8X)	K node location of radial injection.
39	VINJ	8E10.4	Radial injection velocity.
40	EVINJ	8E10.4	Radial injection turbulent kinetic energy.
41	DVINJ	8E10.4	Radial injection turbulence length scale.
42	AVINJ	8E10.4	Radial injection mass flow rate.
43	TVINJ	8E10.4	Radial injection temperature.
44	NSOOT	8(I2,8X)	=0, SOOT calculations not performed; =1, SOOT calculations performed.
	ISOOT		soot calculation started after ERROR falls to SSOOT or after ISOOT number of iterations.
	MPART		Number of soot particle sizes.
			Sip Sets 45-48 if NSOOT=0.
45	SSOOT	8E10.4	See ISOOT.
	AO		Constant a_o in soot nuclei formation rate, equation (6).
	ARCONN		Activation energy divided by gas constant in soot nucleus formation rate, equation (6).
	AAA		Constant a in soot formation rate, equation (8).
	BBB		Constant b in soot formation rate, equation (8).

Card Set	Variable	Format	Description
	FMG		Constant (f-g) in soot nucleus formation rate, equation (7).
	GO		Constant g_o in soot nucleus formation rate, equation (7).
	RHOP		Particle density.
46	PREXPS	8E10.4	Pre-exponent in soot oxidation rate, equation (11).
	ARCONS		Activation energy divided by gas constant in soot oxidation rate, equation (11).
	ALPHA		Temperature exponent in soot oxidation rate, equation (11).
	AAS		Exponent on fuel concentration in soot oxidation rate, equation (11).
	BBS		Exponent on oxygen concentration in soot oxidation rate, equation (11).
	DHR		Heat of fuel combustion reaction.
	CINCP		Incipient carbon/oxygen ratio for soot formation.
	TINCP		soot calculation bypassed if temperature $\leq$TINCP.
47	DPART	8E10.4	soot particle diameters (in microns).
48	FRACP	8E10.4	Relative rates of formation of soot particle sizes.
49	IRAD	I2,8X,	Radiation calculation started after
	SRAD	E10.4	ERROR falls to SRAD or after IRAD number of iterations. (Skip if ITRAD=1).
50	NNOX	3(I2,8X),	=0 NO_x calculations not performed; =1 NO_x calculations performed.
	INOX	2E10.4	NO_x calculations started after ERROR falls to SNOX or after INOX number of iterations.
	ITNOX		Number of iterations of NO_x solution at final iteration of flow solution.
	SNOX		See INOX.
	TNOX		NO_x calculation bypassed if temperature $\leq$ TNOX.

After these 50 card sets, the input to the chemical kinetics program CHEK must be provided. This is described below in Tables B-1, B-2 and B-3.

TABLE B-1. ELEMENTS INPUT CARDS.

Order	Contents	Format	Card Columns
First	ELEMENTS	3A4	1 to 8
Any	One card for each distinct element present in the chemical system. Each card contains:		
	1) Atomic symbol of element--must agree with that used in THERMØ data.	A2	1 to 2
	2) Atomic weight of the element	F10.6	10 to 19
	3) Values of oxidation state of the element (positive, negative or zero).	F10.6	20 to 29
Last	Blank Card	--	--

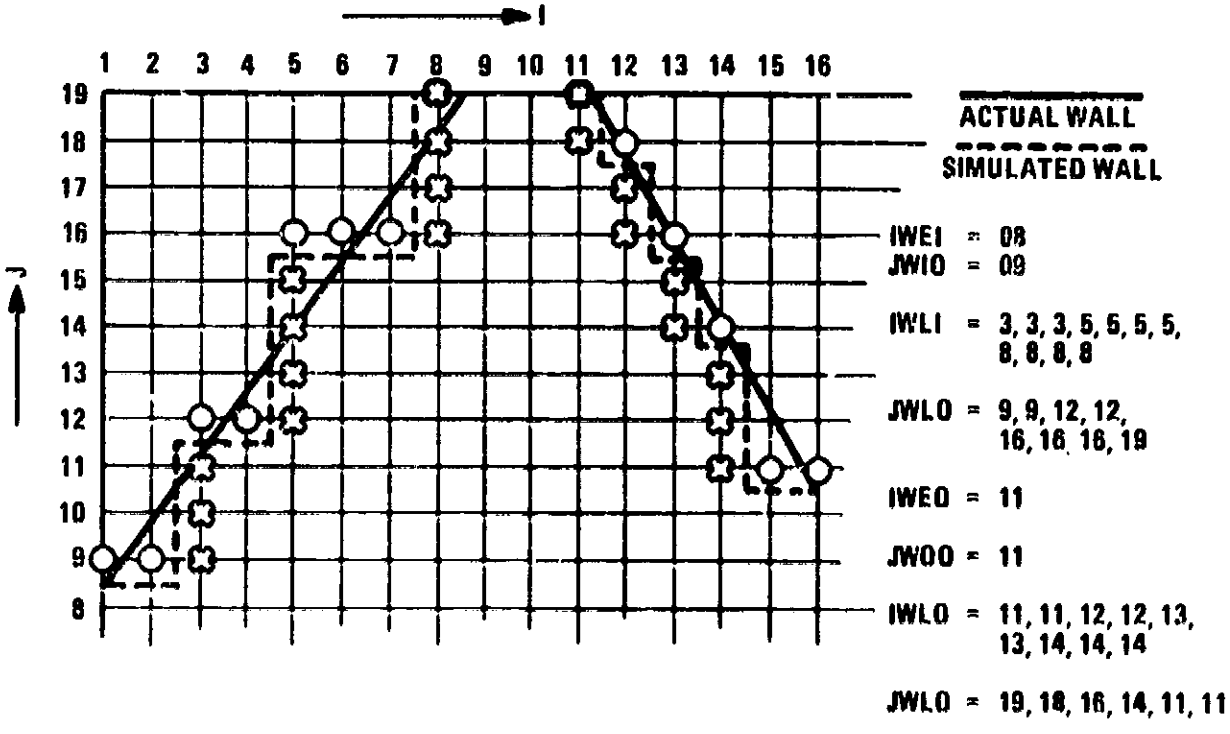

Figure B-1. Definitions of Inclined Wall Indices.

TABLE B-2. THERMØ INPUT CARDS.

Order	Contents	Format	Card Columns
First	THERMØ	3A4	1 to 6
Any	Sets of four cards in sequence for each species in the chemical system. The card formats for each set are, in order:		
First in set	1) Molecular symbol or name of species	3A4	1 to 12
	2) Date	2A3	19 to 24
	3) Atomic Symbols and formula	4(A2,F3.0)	25 to 44
	4) Phase (gas only, letter G)	A1	45
	5) Temperature range, deg K	2F10.3	46 to 65
	6) Integer 1	I15	80
Second in set	1) Coefficients (z_i, i=1,5) for upper temperature range. See Note A.	5E15.8	1 to 75
	2) Integer 2	I5	80
Third in set	1) Coefficients z_6 and z_7 for upper temperature range, and z_3 for lower. See Note A.	5E15.8	1 to 75
	2) Integer 3	I5	80
Fourth in set	1) Coefficients (z_i, i=4,7) for low temperature interval. See Note A.	4E15.8	1 to 60
	2) Integer 4	I20	80
Last	Blank Card	--	--

Note A: The coefficients (z_i, i=1,7) are those which appear in the polynominal expression for the constant pressure specific heat.

TABLE B-3. MECHANISM INPUT CARDS.

Order	Contents	Format	Card Columns
First	MECHANISM	3A4	1 to 9
Any	One card for each distinct forward (or optionally, reverse) reaction step in the mechanism specified. Each card contains:		
	1) Molecular symbols of up to three reactant species. See Note A.	3(2A4)	1 to 24
	2) Molecular symbols of up to three product species. See Note A.	3(2A4)	25 to 48
	3) Exponent B_j. See Notes B and E.	F8.3	49 to 56
	4) Exponent N_j. See Note B	F8.3	57 to 64
	5) Activation temperature T_j, deg K. See Notes B and E.	F8.3	65 to 72
	6) Options:		
	a) for forward reactions, date or comments, etc.	2A4	73 to 80
	b) for reverse reactions, REVERSE. See Note C.	2A4	73 to 79
	c) for global oxidative pyrolysis of hydrocarbon fuels, GLOBAL. See Note D.	2A4	73 to 78
	d) for rate data in cgs units, CGS. See Note E.	--	--
Last	Blank Card	--	--

NOTES:

A. Symbols must be identical to those used in THERMØ data cards.

B. As used in modified Arrhenius expression

$$k_j = 10^{B_j} T^{N_j} \exp(-T_j/T),$$ with units

m^3 kg-mole^{-1} s^{-1} for bimolecular reactions, and

m^6 kg-mole^{-2} s^{-1} for termolecular reactions.

C. If REVERSE is specified, Columns 1 to 48 are ignored. Card with reverse rate data must therefore follow immediately the card with data for the associated forward reaction, and must be in same units.

TABLE B-3. MECHANISM INPUT CARDS (Contd.).

D. All GLOBAL cards must precede other cards in MECHANISM data deck.

E. If CGS is punched in Columns 73-75, B_j must correspond to $cm^3\ gmol^{-1}\ s^{-1}$ or $cm^6\ gmol^{-2}\ s^{-1}$, and T_j must be the activation energy, kcal/gmol.

APPENDIX C

LIST OF FORTRAN VARIABLES

In this appendix a description of the Fortran variables is provided. Table C-1 contains the variables in the 3-D Combustor Program and Table C-2 contains the variables in the chemical kinetics program CREK.

TABLE C-1
LIST OF FORTRAN VARIABLES IN 3-D COMBUSTOR PROGRAM

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
A	STRAD	COEFFICIENT IN TDMA SOLUTION.
AAA	AUX,MAIN	CONSTANT IN SOOT FORMATION (SEE INPUT).
AAS	AUX,MAIN	EXPONENT ON FUEL CONCENTRATION IN SOOT OXIDATION RATE (SEE INPUT).
AA1	AUX,MAIN INIT	EXPONENT ON SPECIES CONCENTRATION IN FIRST STEP OF HYDROCARBON OXIDATION SCHEME.
AA2	AUX,MAIN INIT	EXPONENT ON SPECIES CONCENTRATION IN SECOND STEP OF HYDROCARBON OXIDATION SCHEME.
AA3	AUX,MAIN INIT	EXPONENT ON SPECIES CONCENTRATION IN THIRD STEP OF HYDROCARBON OXIDATION SCHEME.
AA4	AUX,MAIN INIT	EXPONENT ON SPECIES CONCENTRATION IN FOURTH STEP OF HYDROCARBON OXIDATION SCHEME.
ABSOR	MAIN INIT AUXRAD	ABSORPTION COEFFICIENT (IF ITRAD=2).
ABSP	INIT AUX AUXRAD	ARRAY TO STORE ABSORPTION COEFFICIENT.
ALOEF	AUX,DATA	COEFFICIENTS TO LIMIT TEMPERATURE TO ACCOUNT FOR DISSOCIATION.
ACOND	SPRAY	COEFFICIENT IN THERMAL CONDUCTIVITY CALCULATION.
AEXP1	INIT	EXPONENT ON SPECIES CONCENTRATION IN FIRST STEP OF HYDROCARBON OXIDATION SCHEME(=AA1).
AEXP2	INIT	EXPONENT ON SPECIES CONCENTRATION IN SECOND STEP OF HYDROCARBON OXIDATION SCHEME(=AA2).
AEXP3	INIT	EXPONENT ON SPECIES CONCENTRATION IN THIRD STEP OF HYDROCARBON OXIDATION SCHEME(=AA3).
AEXP4	INIT	EXPONENT ON SPECIES CONCENTRATION IN FOURTH STEP OF HYDROCARBON OXIDATION SCHEME(=AA4).
AFSW	MAIN INIT	AIR+FUEL FLOW THROUGH DOME INLET.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
AK	DATA ALLMOD	VON KARMAN CONSTANT.
AKA,AKB	AUX	RATE CONSTANTS IN SOOT OXIDATION EXPRESSION.
AKFAC	MAIN INIT ALLMOD	INTERNALLY DEFINED TURBULENT KINETIC ENERGIES ARE AKFAC TIMES THE APPROPRIATE VELOCITY SQUARED.
AKK,AKT	AUX	RATE CONSTANTS IN SOOT OXIDATION EXPRESSION.
AK2	AUX	RATE CONSTANT IN SOOT OXIDATION EXPRESSION.
AL	INIT	TURBULENCE LENGTH SCALE.
ALFA	MAIN SPRAY	NOZZLE CONE ANGLE.
ALFAC	MAIN INIT ALLMOD	INTERNALLY DEFINED TURBULENT LENGTH SCALES ARE ALFAC TIMES THE APPROPRIATE DISTANCE.
ALIN	INIT	INLET TURBULENCE LENGTH SCALE.
ALNGHT	INIT	LENGTH OF COMBUSTOR.
ALPHA	AUX,MAIN	TEMPERATURE EXPONENT IN SOOT OXIDATION RATE (SEE INPUT).
ALPHAS	AUXRAD	ABSORPTION COEFFICIENT.
ALX,ALXM	STRIDE	CONVECTION FLUX IN X DIRECTION.
ALXP,ALX1	STRIDE	CONVECTION FLUX IN X DIRECTION.
ALY,ALYM	STRIDE	CONVECTION FLUX IN Y DIRECTION.
ALYP,ALY1	STRIDE	CONVECTION FLUX IN Y DIRECTION.
AL2,AL2M	STRIDE	CONVECTION FLUX IN Z DIRECTION.
AL2P,AL21	STRIDE	CONVECTION FLUX IN Z DIRECTION.
AMASS	INIT	TOTAL AIR FLOW RATE.
AMT	SPRAY	FUEL EVAPORATION RATE FOR ONE TIME STEP.
AMU	MAIN AUX ALLMOD	LAMINAR VISCOSITY (SEE INPUT).

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
ANO	AUX	SOOT NUCLEUS FORMATION RATE AT MEAN TEMPERATURE.
ANOO	AUX	SOOT NUCLEUS FORMATION RATE IN FLUID SURROUNDING FINE STRUCTURES.
ANOSTR	AUX	SOOT NUCLEUS FORMATION RATE IN FINE STRUCTURES.
ANUC	ALL	SOOT NUCLEUS CONCENTRATION.
AO	AUX,MAIN	CONSTANT IN SOOT NUCLEUS FORMATION RATE (SEE INPUT).
AP	SOLVE	COEFFICIENT IN TDMA SOLUTION.
APP	SOLVE	COEFFICIENT IN CYCLIC TDMA SOLUTION.
ARCONN	AUX,MAIN	ACTIVATION ENERGY DIVIDED BY GAS CONSTANT IN SOOT NUCLEUS FORMATION RATE (SEE INPUT).
ARCONS	AUX,MAIN	ACTIVATION ENERGY DIVIDED BY GAS CONSTANT IN SOOT OXIDATION RATE (SEE INPUT).
ARCON1	AUX,MAIN INIT	ACTIVATION ENERGY IN FIRST STEP OF HYDROCARBON OXIDATION SCHEME, DIVIDED BY GAS CONSTANT.
ARCON2	AUX,MAIN INIT	ACTIVATION ENERGY IN SECOND STEP OF HYDROCARBON OXIDATION SCHEME, DIVIDED BY GAS CONSTANT.
ARCON3	AUX,MAIN INIT	ACTIVATION ENERGY IN THIRD STEP OF HYDROCARBON OXIDATION SCHEME, DIVIDED BY GAS CONSTANT.
ARCON4	AUX,MAIN INIT	ACTIVATION ENERGY IN FOURTH STEP OF HYDROCARBON OXIDATION SCHEME, DIVIDED BY GAS CONSTANT.
AREA	ALLMOD STRIDE	AREA OF CONTROL VOLUME SURFACE.
AREAT	AUX	SOOT PARTICLE SURFACE AREA.
ARG	AUX	TEMPORARY USAGE.
ARG	SPRAY	SQUARE OF DROPLET DIAMETER.
ARRHEN	AUX	ARRHENIUS REACTION RATE.
AS	SPRAY	DROPLET SURFACE AREA.
ASU	ALLMOD	ABSOLUTE OF CONTINUITY ERROR.
ASUR	CREK	SEE TABLE C-2.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
ASW	INIT	FLOW RATE OF AIR THROUGH DOME INLET.
ASWRLR	INIT	DOME INLET AREA.
AT	SPRAY	QUANTITY USED IN THERMAL CONDUCTIVITY CALCULATION.
AUINJ	MAIN ALLMOD	MASS FLOW RATE THROUGH FILM COOLING SLOT.
AVINJ	MAIN ALLMOD	MASS FLOW RATE THROUGH DILUTION HOLES.
AXM	STRIDE STRAD ALLMOD SOLVE	FINITE-DIFFERENCE COEFFICIENT IN X- DIRECTION.
AXMK	SOLVE	FINITE-DIFFERENCE COEFFICIENT IN X- DIRECTION, USED IN CYCLIC TDMA.
AXP	STRIDE STRAD ALLMOD SOLVE	FINITE-DIFFERENCE COEFFICIENT IN X+ DIRECTION.
AXPK	SOLVE	FINITE-DIFFERENCE COEFFICIENT IN X+ DIRECTION, USED IN CYCLIC TDMA.
AYM	STRIDE STRAD ALLMOD SOLVE	FINITE-DIFFERENCE COEFFICIENT IN Y- DIRECTION.
AYMK	SOLVE	FINITE-DIFFERENCE COEFFICIENT IN Y- DIRECTION, USED IN CYCLIC TDMA.
AYP	STRIDE STRAD ALLMOD SOLVE	FINITE-DIFFERENCE COEFFICIENT IN Y+ DIRECTION.
AYPK	SOLVE	FINITE-DIFFERENCE COEFFICIENT IN Y+ DIRECTION, USED IN CYCLIC TDMA.
AZM	STRIDE STRAD ALLMOD SOLVE	FINITE-DIFFERENCE COEFFICIENT IN Z- DIRECTION.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
AZMK	SOLVE	FINITE-DIFFERENCE COEFFICIENT IN Z- DIRECTION, USED IN CYCLIC TDMA.
AZP	STRIDE STRAD ALLMOD SOLVE	FINITE-DIFFERENCE COEFFICIENT IN Z+ DIRECTION.
AZPK	SOLVE	FINITE-DIFFERENCE COEFFICIENT IN Z+ DIRECTION, USED IN CYCLIC TDMA.
A1-A6	AUX	TEMPORARY USAGE.
A4	INIT	TEMPORARY USAGE OF FLOW AREA.
B	STRAD	COEFFICIENT IN TDMA SOLUTION.
BBB	AUX,MAIN	CONSTANT IN SOOT FORMATION (SEE INPUT).
BBS	AUX,MAIN INIT	EXPONENT ON O2 CONCENTRATION IN SOOT OXIDATION RATE (SEE INPUT).
BB1	AUX,MAIN INIT	EXPONENT ON SPECIES CONCENTRATION IN FIRST STEP OF HYDROCARBON OXIDATION SCHEME.
BB2	AUX,MAIN INIT	EXPONENT ON SPECIES CONCENTRATION IN SECOND STEP OF HYDROCARBON OXIDATION SCHEME.
BB3	AUX,MAIN INIT	EXPONENT ON SPECIES CONCENTRATION IN THIRD STEP OF HYDROCARBON OXIDATION SCHEME.
BB4	AUX,MAIN INIT	EXPONENT ON SPECIES CONCENTRATION IN FOURTH STEP OF HYDROCARBON OXIDATION SCHEME.
BCOND	SPRAY	COEFFICIENT IN THERMAL CONDUCTIVITY CALCULATION.
BEE	SPRAY	DRIVING FORCE FOR MASS TRANSFER.
BETA	MAIN SPRAY	NOZZLE BACK ANGLE.
BEXP1	INIT	EXPONENT ON SPECIES CONCENTRATION IN FIRST STEP OF HYDROCARBON OXIDATION SCHEME(=BB1).
BEXP2	INIT	EXPONENT ON SPECIES CONCENTRATION IN SECOND STEP OF HYDROCARBON OXIDATION SCHEME(=BB2).
BEXP3	INIT	EXPONENT ON SPECIES CONCENTRATION IN THIRD STEP OF HYDROCARBON OXIDATION SCHEME(=BB3).

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
BEXP4	INIT	EXPONENT ON SPECIES CONCENTRATION IN FOURTH STEP OF HYDROCARBON OXIDATION SCHEME(=BR4).
BK	SOLVE	TEMPORARY USAGE.
BP	SOLVE	COEFFICIENT IN TDMA SOLUTION.
BPP	SOLVE	COEFFICIENT IN CYCLIC TDMA SOLUTION.
BT	SPRAY	QUANTITY USED IN THERMAL CONDUCTIVITY CALCULATION.
CANG	MAIN	CONSTANT TO CONVERT UNITS ON ANGLES.
CARB	AUX	MASS FRACTION OF ELEMENTAL CARBON.
CC1	AUX,MAIN INIT	EXPONENT ON SPECIES CONCENTRATION IN FIRST STEP OF HYDROCARBON OXIDATION SCHEME.
CC2	AUX,MAIN INIT	EXPONENT ON SPECIES CONCENTRATION IN SECOND STEP OF HYDROCARBON OXIDATION SCHEME.
CC3	AUX,MAIN INIT	EXPONENT ON SPECIES CONCENTRATION IN THIRD STEP OF HYDROCARBON OXIDATION SCHEME.
CC4	AUX,MAIN INIT	EXPONENT ON SPECIES CONCENTRATION IN FOURTH STEP OF HYDROCARBON OXIDATION SCHEME.
CD	AUX ALLMOD	CONSTANT IN TURBULENCE MODEL.
CDS,CD1	SPRAY	DROPLET DRAG COEFFICIENT.
CEBU1	INIT	EDDY-BREAK-UP CONSTANT FOR FIRST STEP OF HYDROCARBON OXIDATION SCHEME.
CEBU2	INIT	EDDY-BREAK-UP CONSTANT FOR SECOND STEP OF HYDROCARBON OXIDATION SCHEME.
CEBU3	INIT	EDDY-BREAK-UP CONSTANT FOR THIRD STEP OF HYDROCARBON OXIDATION SCHEME.
CEBU4	INIT	EDDY-BREAK-UP CONSTANT FOR FOURTH STEP OF HYDROCARBON OXIDATION SCHEME.
CENER	MAIN	CONSTANTS TO CONVERT UNITS ON ENERGY.
CEXP1	AUX,INIT	EXPONENT ON SPECIES CONCENTRATION IN FIRST STEP OF HYDROCARBON OXIDATION SCHEME(=CC1).

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
CEXP2	AUX,INIT	EXPONENT ON SPECIES CONCENTRATION IN SECOND STEP OF HYDROCARBON OXIDATION SCHEME(=CC2).
CEXP3	AUX,INIT	EXPONENT ON SPECIES CONCENTRATION IN THIRD STEP OF HYDROCARBON OXIDATION SCHEME(=CC3).
CEXP4	AUX,INIT	EXPONENT ON SPECIES CONCENTRATION IN FOURTH STEP OF HYDROCARBON OXIDATION SCHEME(=CC4).
CFR	ALLMOD AUX INIT	SKIN FRICTION COEFFICIENT.
CINCP	AUX,MAIN	INCIPIENT CARBON/OXYGEN RATIO FOR SOOT FORMATION.
CK	SOLVE	TEMPORARY USAGE.
CLEND	MAIN	CONSTANTS TO CONVERT UNITS ON LENGTHS.
CLENV	MAIN	CONSTANTS TO CONVERT UNITS ON VELOCITIES.
CMASS	MAIN	CONSTANTS TO CONVERT UNITS ON MASS.
CNO	OUTPUT	NOX EMISSIONS INDEX.
COND1	SPRAY	THERMAL CONDUCTIVITY OF FUEL VAPORS.
CONS	SPRAY	TEMPORARY USAGE.
CONS2	AUX	TEMPORARY USAGE.
CON2	SPRAY	FRACTION OF FUEL EVAPORATED.
COSA	SPRAY	COSINE OF HALF THE NOZZLE CONE ANGLE.
COSB	SPRAY	COSINE OF NOZZLE BACK ANGLE.
COSD	SPRAY	COSINE OF NOZZLE DOWN ANGLE.
COST	SPRAY	COSINE OF CURRENT SPRAY CONE SEGMENT ANGLE.
CP	AUX ALLMOD	CONSTANT PRESSURE SPECIFIC HEAT.
CPI	INIT AUX	CONSTANT PRESSURE SPECIFIC HEAT.
CPLF	SPRAY	SPECIFIC HEAT OF LIQUID DROPLET.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
CPR	AUX	CONSTANT PRESSURE SPECIFIC HEAT.
CPRESS	MAIN	CONSTANTS TO CONVERT UNITS ON PRESSURE.
CPSUM	ALLMOD AUX	CONSTANT PRESSURE SPECIFIC HEAT OF GAS MIXTURE.
CP1	SPRAY	SPECIFIC HEAT.
CR1	AUX,MAIN	EDDY-BREAK-UP CONSTANT IN FIRST STEP OF HYDROCARBON OXIDATION SCHEME(=CEBU1).
CR2	AUX,MAIN	EDDY-BREAK-UP CONSTANT IN SECOND STEP OF OF HYDROCARBON OXIDATION SCHEME(=CEBU2).
CR3	AUX,MAIN	EDDY-BREAK-UP CONSTANT IN THIRD STEP OF HYDROCARBON OXIDATION SCHEME(=CEBU3).
CR4	AUX,MAIN	EDDY-BREAK-UP CONSTANT IN FOURTH STEP OF HYDROCARBON OXIDATION SCHEME(=CEBU4).
CSMD	OUTPUT	SMOKE EMISSIONS INDEX.
CTEMP	MAIN	CONSTANT TO CONVERT UNITS ON TEMPERATURE.
CX	STRIDE	TEMPORARY STORAGE FOR CONVECTIVE/DIFFUSIVE FLUX IN X DIRECTION.
CXU,CXUP	STRIDE	TEMPORARY STORAGE FOR CONVECTIVE FLUX IN X DIRECTION.
CXX	INIT AUX MAIN	NUMBER OF CARBON ATOMS IN THE FUEL.
CY	STRIDE	TEMPORARY STORAGE FOR CONVECTIVE/DIFFUSIVE FLUX IN Y DIRECTION.
CYP		NOT USED.
CYU,CYUP	STRIDE	TEMPORARY STORAGE FOR CONVECTIVE FLUX IN Y DIRECTION.
CZ	STRIDE	TEMPORARY STORAGE FOR CONVECTIVE/DIFFUSIVE FLUX IN Z DIRECTION.
CZP		NOT USED.
CZU,CZUP	STRIDE	TEMPORARY STORAGE FOR CONVECTIVE FLUX IN Z DIRECTION.
C1	AUX,MAIN	CONSTANT IN TURBULENCE MODEL.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
C2	AUX, MAIN	CONSTANT IN TURBULENCE MODEL.
DANG	SPRAY	DELTA(ANGLE).
DELTA	SPRAY MAIN	FUEL NOZZLE DOWN ANGLE.
DELTAT	AUX	TEMPERATURE RISE.
DEN	AUX, MAIN	DENSITY (SEE INPUT).
DENOM	SOLVE	TEMPORARY USAGE.
DENST	AUX	DENSITY.
DENSTY	STRIDE	DENSITY.
DEVAP	SPRAY	FRACTION OF FUEL EVAPORATED IN ONE TIME STEP.
DFAC	MAIN STRIDE	QUANTITY USED TO GRADUALLY INTRODUCE 2 DIRECTION DIFFUSION.
DFTW	TSOLVE	DIFFERENTIAL OF HEAT TRANSFER W.R.T. TEMPERATURE.
DHR	AUX, MAIN	HEAT OF FUEL COMBUSTION REACTION.
DIA	SPRAY	INSTANTANEOUS DROPLET DIAMETER.
DIAO	SPRAY	INITIAL DROPLET DIAMETER.
DIST	ALLMOD AUX STRIDE	INTERNODAL DISTANCE.
DIVG	STRIDE ALLMOD	MASS IMBALANCE AT A CONTROL VOLUME.
DK	SOLVE	TEMPORARY USAGE.
DLIM	SPRAY	CONSTANT TO LIMIT TIME STEP.
DM	SPRAY	DROPLET MASS.
DMDOT	OUTPUT	MASS FLOW RATE.
DP	SOLVE	COEFFICIENT IN CYCLIC TDMA SOLUTION.
DPART	AUX, MAIN	SOOT PARTICLE DIAMETERS.

C-2

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
DQCH	TSOLVE	HEAT TRANSFER COEFFICIENT.
DQRH	TSOLVE	DIFFERENTIAL OF RADIATION HEAT TRANSFER W.R.T. TEMPERATURE.
DRHODP	STPIDE	PARTIAL DERIVATIVE OF DENSITY W.R.T. PRESSURE.
DSDCO	AUX	TEMPORARY USAGE IN CO SOURCE TERM.
DSDFU	AUX	TEMPORARY USAGE IN FUEL SOURCE TERM.
DSDH	AUX	TEMPORARY USAGE IN ENTHALPY SOURCE TERM.
DSDOT	OUTPUT	TEMPORARY USAGE.
DSDSP	AUX	TEMPORARY USAGE IN CXHY-2 AND H2 SOURCE TERMS.
DSMD	SPRAY	RATIO OF DROPLET DIAMETER TO SMD.
DT	STRIDE	TIME INCREMENT.
DTF	SPRAY	TEMPERATURE RISE OF DROPLET.
DTHETA	SPRAY	DIFFERENCE BETWEEN INITIAL AND FINAL SPRAY CONE SEGMENT ANGLES.
DTI	SPRAY	LIMIT ON TIME STEP TO AVOID NUMERICAL INSTABILITY.
DTI1-7	SPRAY	LIMITS ON TIME STEP TO AVOID NUMERICAL INSTABILITY.
DU	STRIDE SOLVE AUX	PRESSURE-VELOCITY COEFFICIENT FOR U-VELOCITY.
DUDXM	AUX	PARTIAL DERIVATIVE OF U W.R.T. X AT I LOCATION.
DUDXP	AUX	PARTIAL DERIVATIVE OF U W.R.T. X AT I+1 LOCATION.
DUDYM	AUX	PARTIAL DERIVATIVE OF U W.R.T. Y AT I LOCATION.
DUDYP	AUX	PARTIAL DERIVATIVE OF U W.R.T. Y AT I+1 LOCATION.
DUDZM	AUX	PARTIAL DERIVATIVE OF U W.R.T. Z AT I LOCATION.
DUDZP	AUX	PARTIAL DERIVATIVE OF U W.R.T. Z AT I+1 LOCATION.
DUIDXJ	AUX	PARTIAL DERIVATIVE OF UI W.R.T. XJ.
DV	STRIDE SOLVE AUX	PRESSURE-VELOCITY COEFFICIENT FOR V-VELOCITY.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
DVDXM	AUX	PARTIAL DERIVATIVE OF V W.R.T. X AT J LOCATION.
DVDXP	AUX	PARTIAL DERIVATIVE OF V W.R.T. X AT J+1 LOCATION.
DVDY	AUX	VELOCITY GRADIENT NEAR A WALL.
DVDYM	AUX	PARTIAL DERIVATIVE OF V W.R.T. Y AT J LOCATION.
DVDYP	AUX	PARTIAL DERIVATIVE OF V W.R.T. Y AT J+1 LOCATION.
DVDZM	AUX	PARTIAL DERIVATIVE OF V W.R.T. Z AT J LOCATION.
DVDZP	AUX	PARTIAL DERIVATIVE OF V W.R.T. Z AT J+1 LOCATION.
DVINJ	INIT PAIN	RADIAL INJECTION TURBULENCE LENGTH SCALE.
DW	STRIDE SOLVE AUX ALLMOD	PRESSURE-VELOCITY COEFFICIENT FOR W-VELOCITY.
DWDXM	AUX	PARTIAL DERIVATIVE OF W W.R.T. X AT K LOCATION.
DWDXP	AUX	PARTIAL DERIVATIVE OF W W.R.T. X AT K+1 LOCATION.
DWDYM	AUX	PARTIAL DERIVATIVE OF W W.R.T. Y AT K LOCATION.
DWDYP	AUX	PARTIAL DERIVATIVE OF W W.R.T. Y AT K+1 LOCATION.
DWDZM	AUX	PARTIAL DERIVATIVE OF W W.R.T. Z AT K LOCATION.
DWDZP	AUX	PARTIAL DERIVATIVE OF W W.R.T. Z AT K+1 LOCATION.
DX	AUX	INTERNODAL DISTANCE IN X DIRECTION.
DX	SPRAY	DISTANCE TRAVELED BY DROPLET IN X DIRECTION.
DY	INIT AUX	INTERNODAL DISTANCE IN Y DIRECTION.
DY	SPRAY	DISTANCE TRAVELED BY DROPLET IN Y DIRECTION.
DZ	AUX INIT	INTERNODAL DISTANCE IN Z DIRECTION.
DZ	SPRAY	DISTANCE TRAVELED BY DROPLET IN Z DIRECTION.
E	ALLMOD DATA	CONSTANT E IN LOG-LAW OF THE WALL.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
EDK	STRIDE AUX	DISSIPATION DIVIDED BY TURBULENCE ENERGY.
EDKIJ	STRIDE	DISSIPATION DIVIDED BY TURBULENCE ENERGY AT NODE I,J,K.
EDK2	AUX	DISSIPATION DIVIDED BY TURBULENCE ENERGY SQUARED.
EE	SPRAY	CONSTANT IN DROPLET BOILING POINT CALCULATION.
EMDOT	AUX	RATE OF MASS TRANSFER BETWEEN FINE STRUCTURES AND SURROUNDING FLUID.
EMDOTR	AUX	TEMPORARY USAGE.
EMI	INIT AUX *SOLVE ALLMOD	=EMISW/(2.0-EMISW).
EMISIN	INIT	INLET EMISSIVITY.
EMISR	INIT ALLMOD	GAS EMISSIVITY.
EMISW	ALLMOD INIT	WALL EMISSIVITY.
EMPIN	AUX	TEMPORARY USAGE.
EMP	AUX	MASS OF SOOT PARTICLE.
EMPR	AUX	MASS FRACTION OF PRODUCTS.
EMV	STRIDE	TOTAL CONVECTIVE AND DIFFUSIVE MASS INFLOW INTO A FINITE-DIFFERENCE CELL, SEE TABLE C-2.
ENN	AUX	MEAN SOOT PARTICLE CONCENTRATION.
ENND	AUX	SOOT PARTICLE CONCENTRATION IN FLUID SURROUNDING FINE STRUCTURES.
ENNRHO	AUX	ENN DIVIDED BY GAS DENSITY.
ENNSTR	AUX	SOOT PARTICLE CONCENTRATION IN FINE STRUCTURES.
END	AUX	SOOT NUCLEUS CONCENTRATION IN FLUID SURROUNDING FINE STRUCTURES.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
ENRHO	AUX	MEAN SOOT NUCLEUS CONCENTRATION DIVIDED BY GAS DENSITY.
ENSTP	AUX	SOOT NUCLEUS CONCENTRATION IN FINE STRUCTURES.
ENSTR1	AUX	TEMPORARY USAGE.
ENSTR2	AUX	TEMPORARY USAGE.
EP	SOLVE	COEFFICIENT IN CYCLIC TDMA SOLUTION.
FR	CREK	EQUIVALENCE RATIO. SEE TABLE C-2.
ERROR	MAIN	PROGRAM WILL TERMINATE IF TOTAL ERROR IN MASS BECOMES LESS THAN THIS VALUE.
ER1	INIT	ACTIVATION ENERGY FOR THE FIRST STEP OF HYDROCARBON OXIDATION SCHEME, DIVIDED BY GAS CONSTANT (=ARCON1).
ER2	INIT	ACTIVATION ENERGY FOR THE SECOND STEP OF HYDROCARBON OXIDATION SCHEME, DIVIDED BY GAS CONSTANT (=ARCON2).
ER3	INIT	ACTIVATION ENERGY FOR THE THIRD STEP OF HYDROCARBON OXIDATION SCHEME, DIVIDED BY GAS CONSTANT (=ARCON3).
ER4	INIT	ACTIVATION ENERGY FOR THE FOURTH STEP OF HYDROCARBON OXIDATION SCHEME, DIVIDED BY GAS CONSTANT (=ARCON4).
ET	SPRAY	VARIABLE IN DROPLET BOILING POINT CALCULATION.
EVAP	SPRAY ALLMOD STRIDE	EVAPORATION RATE OF LIQUID FUEL.
EVAPI-M	SPRAY	INTERPHASE MOMENTUM TRANSFER IN X, Y, Z DIRECTIONS.
EVINJ	INIT MAIN	RADIAL INJECTION TURBULENCE ENERGY.
EVSU	SPRAY ALLMOD	ARRAY USED TO STORE INTERPHASE MOMENTUM TRANSFER.
F	ALL	ARRAY USED TO STORE DEPENDENT VARIABLES.
FAC	SPRAY	TEMPORARY USAGE.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
FACP	AUXRAD	TEMPORARY USAGE.
FAV	AUX	AVERAGE RADIATION FLUX.
FCH	ALL	INTERMEDIATE HYDROCARBON CONCENTRATION.
FDFU		NOT USED.
FEND	SOLVE	QUANTITY USED IN CYCLIC TDMA.
FEVAP	SPRAY	FRACTION OF FUEL EVAPORATED.
FEXIT	INIT	UNBURNT FUEL MASS FRACTION.
FH2	ALL	HYDROGEN MASS FRACTION.
FK	INIT	INLET TURBULENCE KINETIC ENERGY.
FKFU		NOT USED.
FLO	INIT	FLOW RATE AT EACH AXIAL STATION.
FLOW	OUTPUT	MASS FLOW RATE.
FLOWIN	INIT ALLMOD	INLET MASS FLOW RATE.
FLOWOT	ALLMOD	FLOW RATE AT EXIT PLANE.
FLPCO2	INIT AUX AUXRAD	CO2 MASS FRACTION.
FLPE	AUX AUXRAD	EMISSIVE POWER.
FLPH2O	INIT AUX AUXRAD	H2O MASS FRACTION.
FLPN2	INIT AUX AUXRAD	N2 MASS FRACTION.
FLPOX	INIT AUX AUXRAD SPRAY	O2 MASS FRACTION.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
FLPTE	AUX AUXRAD	TEMPERATURE.
FLZP	SOLVE	F VALUE AT NODE LZP.
FMA		NOT USED.
FMG	AUX, MAIN	CONSTANT IN SOOT NUCLEUS FORMATION RATE (SEE INPUT).
FMGF	AUX	TEMPORARY USAGE.
FQ	CREK	SEE TABLE C-2.
FRACP	AUX, MAIN	RELATIVE RATES OF FORMATION OF SOOT PARTICLE SIZES.
FRACT	SPRAY	CUMULATIVE MASS FRACTION OF DROPLETS IN DIFFERENT SIZE GROUPS.
FS	ALL	ARRAY USED TO STORE SPECIES MASS FRACTIONS.
FSLP	STRIDE	TEMPORARY STORAGE FOR FS(LP).
FST	INIT	STOICHIOMETRIC VALUE OF MIXTURE FRACTION.
FSTOIC	INIT AUX	STOICHIOMETRIC VALUE OF MIXTURE FRACTION.
FSW	INIT MAIN	FLOW RATE OF FUEL THROUGH DOME INLET.
FTW	TSOLVE	RADIATIVE+CONVECTIVE HEAT TRANSFER.
FUARAT	INIT	FUEL/AIR RATIO.
FUB	INIT AUX AUXRAD	MASS FRACTION OF BURNT FUEL.
FUEL	INIT	FUEL FLOW RATE AT EACH AXIAL STATION.
FUFLF	INIT	MASS FRACTION OF UNBURNT FUEL.
FUFLI	INIT	MIXTURE FRACTION.
FUELS	INIT	LIQUID FUEL FLOW RATE AT EACH AXIAL STATION.
FUMCO	INIT MAIN	INITIAL ESTIMATE OF CO MASS FRACTION.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
FUMSW	INIT	FUEL/AIR RATIO AT DOME INLET.
FUOX	INIT	MIXTURE FRACTION AT EACH AXIAL STATION.
FUOXSW	INIT	MIXTURE FRACTION AT DOME INLET.
FUT	STRIDE	MIXTURE FRACTION.
FUTOT	INIT	TOTAL FUEL FLOW RATE.
FX	SPRAY	DRAG FORCE ON DROPLET IN X DIRECTION.
FXM	ALL	INTERPOLATION FACTOR FOR X- DIRECTION NODAL DISTANCES.
FXP	ALL	INTERPOLATION FACTOR FOR X+ DIRECTION NODAL DISTANCES.
FY	SPRAY	DRAG FORCE ON DROPLET IN Y DIRECTION.
FYM	ALL	INTERPOLATION FACTOR FOR Y- DIRECTION NODAL DISTANCES.
FYP	ALL	INTERPOLATION FACTOR FOR Y+ DIRECTION NODAL DISTANCES.
FZ	SPRAY	DRAG FORCE ON DROPLET IN Z DIRECTION.
FZM	ALL	INTERPOLATION FACTOR FOR Z- DIRECTION NODAL DISTANCES.
FZP	ALL	INTERPOLATION FACTOR FOR Z+ DIRECTION NODAL DISTANCES.
GAM	ALL	DIFFUSION COEFFICIENT.
GAMAS	AUX	MASS FRACTION OF FLUID IN FINE STRUCTURES.
GAMDDL	ALLMOD	TEMPORARY USAGE.
GAMLP	AUX STRIDE	DIFFUSION COEFFICIENT AT NODE LP.
GAMLXM	AUX	DIFFUSION COEFFICIENT AT NODE LXM.
GAMLYM	AUX	DIFFUSION COEFFICIENT AT NODE LYM.
GAMLZM	AUX	DIFFUSION COEFFICIENT AT NODE LZM.
GAMM	AUX	AVERAGE DIFFUSION COEFFICIENT.
GAMP	AUX	AVERAGE DIFFUSION COEFFICIENT.
GAMPT2	AUX	AVERAGE DIFFUSION COEFFICIENT.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
GASCON	AUX,MAIN	UNIVERSAL GAS CONSTANT DIVIDED BY MOLECULAR WEIGHT OF AIR.
GENR	AUX	GENERATION RATE OF TURBULENCE ENERGY.
GO	AUX,MAIN	CONSTANT IN SOOT NUCLEUS FORMATION RATE (SEE INPUT).
GPSI	AUX	=GAMAS*PSI.
GPSIP	AUX	GPSI DIVIDED BY DENSITY OF FINE STRUCTURES.
H	ALL	ENTHALPY.
HCO	INIT	HEAT OF COMBUSTION OF CO.
HCRAT	INIT	TEMPORARY USAGE.
HDREF	ALLMOD	TEMPORARY USAGE.
HEIGHT	INIT	CHANNEL HEIGHT OF COMBUSTOR.
HEVAP	SPRAY	HEAT OF VAPORIZATION OF LIQUID FUEL.
HFU	MAIN INIT	HEAT OF FORMATION OF FUEL.
HFUEL	SPRAY	HEAT OF COMBUSTION OF FUEL.
HPI	ALLMOD AUX INIT	TEMPORARY USAGE FOR ENTHALPY.
HSURC	STRIDE	MIXTURE ENTHALPY.
HSUM	AUX ALLMOD INIT STRIDE	ENTHALPY OF GAS MIXTURE.
HT	SPRAY	HEAT TRANSFER COEFFICIENT FOR DROPLET HEATUP.
HTC	ALLMOD AUX	HEAT TRANSFER COEFFICIENT.
HTCEXT		EXTERNAL HEAT TRANSFER COEFFICIENT (NOT USED).
HTCI	TSOLVE	HEAT TRANSFER COEFFICIENT.
HYY	INIT MAIN AUX	NUMBER OF HYDROGEN ATOMS IN FUEL.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
H1,H2	INIT	ENTHALPY(TEMPORARY USAGE).
I8	SPRAY	INDEX TO DENOTE LOCATION OF I BOUNDARY.
ICONVG	STRIDE	=0,CHEMICAL KINETICS SOLUTION NOT CONVERGED. =1,CHEMICAL KINETICS SOLUTION CONVERGED.
ICTDMA	SOLVE PAIN	NUMBER OF SWEEPS FOR EACH VARIABLE IN SOLVE (SEE INPUT).
IDCH	DATA,INIT AUX	INDEX FOR INTERMEDIATE HYDROCARBON MASS FRACTION.
IDCO	DATA,INIT AUX	INDEX FOR CO MASS FRACTION.
IDCO2	DATA,INIT AUX	INDEX FOR CO2 MASS FRACTION.
IDFU	DATA,INIT AUX SPRAY STRIDE ALLMOD	INDEX FOR FUEL MASS FRACTION.
IDH1	DATA	INDEX FOR H ATOM MASS FRACTION.
IDH2	DATA,INIT AUX	INDEX FOR H2 MASS FRACTION.
IDH2O	DATA,INIT AUX	INDEX FOR H2O MASS FRACTION.
IDK	AUX	=01 FOR RATE CONTROLLED COMBUSTION. =02 FOR MIXING CONTROLLED COMBUSTION.
IDNO	DATA	INDEX FOR NO MASS FRACTION.
IDNO2	DATA	INDEX FOR NO2 MASS FRACTION.
IDN1	DATA	INDEX FOR N ATOM MASS FRACTION.
IDN2	DATA,INIT ALLMOD AUX STRIDE	INDEX FOR N2 MASS FRACTION.
IDO	DATA	INDEX FOR O ATOM MASS FRACTION.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
IDOH	DATA	INDEX FOR OH MASS FRACTION.
IDO2	DATA, INIT ALLMOD UX STRIDE	INDEX FOR O2 MASS FRACTION.
IDW	MAIN ALLMOD STRIDE AUX	TYPE OF BOUNDARY AT J=1(SEE INPUT).
IE	ALL	ENDING VALUE OF I(LOCAL VALUE OF IWLO).
IEND	FPRINT	ENDING VALUE OF I FOR PRINTOUT.
IG	SPRAY	DO-LOOP INDEX FOR DROPLET SIZE GROUPS.
IGAM1-2	DATA ALLMOD	INDEX TO DENOTE TYPE OF BOUNDARY CONDITION FOR A DEPENDENT VARIABLE.
IGPNT	SPRAY	INDEX FOR DIAGNOSTIC PRINTOUT.
IHCPS	HCPS	INDEX FOR CALCULATING THERMODYNAMIC PROPERTIES.
IJUMP	OUTPUT MAIN	NUMBER OF ITERATIONS BETWEEN PRINTOUT.
IKIN	INIT ALLMOD AUX STRIDE	INDEX FOR BOUNDARY CONDITIONS.
IL	STRIDE	TEMPORARY USAGE.
IL	SPRAY	DO-LOOP INDEX FOR DROPLET RAYS.
ILC	CREK	SEE TABLE C-2.
ILH	CREK	SEE TABLE C-2.
ILOC	SPRAY	I INDEX FOR DROPLET LOCATION.
IMAT	CREK	SEE TABLE C-2.
IMAX	MAIN ALLMOD	I LOCATION OF MAXIMUM CONTINUITY ERROR.
INCOMP		INDEX TO DENOTE COMPRESSIBILITY(NOT USED).

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINETION
IND	STRIDE	INDEX USED IN RADIATION CALCULATIONS.
INDX	ALLMOD	=1 IF U VELOCITY IS NEGATIVE AT EXIT, OTHERWISE =0.
INDX	SPRAY	INDEX FOR TYPE OF BOUNDARY.
IND	SOLVE	DO-LOOP INDEX.
INDMAX	SOLVE	NUMBER OF TDMA SWEEPS.
INOX	MAIN STRIDE	INDEX TO DECIDE ON NOX CALCULATIONS(SEE SNOX).
INTAPE	MAIN	INDEX FOR INITIAL FIELD PRINTOUT(SEE INPUT).
INV	INIT STRIDE	TEMPORARY USAGE.
IOLD	SPRAY	PREVIOUS I LOCATION OF DROPLET.
IONE	FPRINT	FIRST VALUE OF I FOR PRINTOUT.
IP	STRIDE	TEMPORARY USAGE.
IPAR	MAIN STRIDE	INDEX FOR ABSOLUTE OR RELATIVE PRESSURE(SEE INPUT).
IPLAX	MAIN STRIDE	INDEX FOR PLANE OR AXISYMMETRIC FLOW(SEE INPUT).
IPRINT	FPRINT MAIN	INDEX FOR PRINTOUT OF DEPENDENT VARIABLES (SEE INPUT).
IRAD	MAIN	INDEX FOR RADIATION SOLUTION(SEE SRAD).
IREF	MAIN	I LOCATION OF REFERENCE PRESSURE LOCATION.
IRES	MAIN INIT STRIDE AUX	INDEX FOR RESTARTING SOLUTION(SEE INPUT).
IS	ALL	STARTING VALUE OF I(LOCAL VALUE OF IWLI).
ISOLVE	STRIDE MAIN AUX	INDEX FOR SOLUTION OF DEPENDENT VARIABLES (SEE INPUT).

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
ISOOT	MAIN	INDEX FOR SOOT SOLUTION(SEE SSOOT).
ISP	MAIN	TEMPORARY USAGE.
ISPRAY	MAIN	NUMBER OF ITERATIONS BETWEEN SPRAY SOLUTIONS.
ISTART	FPRINT	STARTING VALUE OF I FOR PRINTOUT.
ISTEP	MAIN STRIDE AUX OUTPUT	NUMBER OF CURRENT ITERATION.
ISTOP	FPRINT	ENDING DEPENDENT VARIABLE INDEX FOR PRINTOUT.
ISTR	STRIDE	FIRST I LOCATION.
ISTRT	FPRINT	STARTING DEPENDENT VARIABLE INDEX FOR PRINTOUT.
ISTR1	SOLVE STRAD	=IS-1.
ISTUN		INDEX FOR STEADY/UNSTEADY FLOW(NOT USED).
ISUP	SOLVE	=ISTR+1.
ISUN	STRAD	=IS+IE.
ISUM1	SOLVE	=IS+IE.
ISWP	SOLVE STRIDE	INDEX USED FOR Y-TDMA SWEEP DIRECTION.
ITER	CREK	NUMBER OF CURRENT ITERATION OF CREK SOLUTION.
ITNOX	STRIDE MAIN	NUMBER OF ITERATIONS OF NOX SOLUTION AT FINAL ITERATION OF FLOW SOLUTION.
ITR	STRIDE	NUMBER OF CHEMICAL KINETICS ITERATIONS.
ITR	TSOLVE	=1 IF RADIATION IGNORED, =2 IF RADIATION CONSIDERED.
ITRAD	TSOLVE MAIN AUX	INDEX FOR RADIATION SOLUTION(SEE INPUT).
ITWALL	AUX	INDEX FOR WALL TEMPERATURE SOLUTION(SEE INPUT).
ITYPE	SPRAY	=1 FOR HEATING DROPLET, =2 FOR BOILING DROPLET.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
IU	MAIN	INDEX FOR TYPE OF UNITS (SEE INPUT).
IU	SPRAY	=IUINJ-1.
IUINJ	ALLMOD MAIN INIT	I NODE LOCATION OF COOLING SLOTS.
IVINJ	INIT MAIN ALLMOD	I NODE LOCATION OF RADIAL INJECTION HOLES.
IWEI	MAIN	I NODE AT WHICH UPSTREAM INCLINED WALL ENDS.
IWEO	MAIN	I NODE AT WHICH DOWNSTREAM INCLINED WALL STARTS.
IWLI	ALL	STARTING I NODES OF CALCULATION DOMAIN WHEN INCLINED WALL IS PRESENT.
IWLO	ALL	ENDING I NODES OF CALCULATION DOMAIN WHEN INCLINED WALL IS PRESENT.
IXY	SOLVE STRIDE	INDEX FOR DIRECTION OF TDMA SWEEPS.
JB	SPRAY	INDEX TO DENOTE LOCATION OF J BOUNDARY.
JE	ALL	LOCAL VALUE OF JWLO-1.
JJ	INIT	TEMPORARY USAGE.
JJ	SOLVE STRAD	DO-LOOP INDEX.
JJJ	STRIDE	NUMBER OF REACTION STEPS (JJ OF CRIK, SEE TABLE C-21.
JKIN	INIT ALLMOD AUX STRIDE	INDEX FOR TYPE OF BOUNDARY.
JL	STRIDE	TEMPORARY USAGE.
JLOC	SPRAY	J LOCATION OF DROPLET.
JM	ALL	=(J-1)*IMAX.
JMAX	MAIN ALLMOD	J LOCATION OF MAXIMUM CONTINUITY ERROR.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
JNOX	MAIN	TEMPORARY USAGE.
JOLD	SPRAY	PREVIOUS J LOCATION OF DROPLET.
JONE	FPRINT	FIRST J VALUE FOR PRINTOUT.
JP	STRIDE	TEMPORARY USAGE.
JPLANE	AUXRAD STRAD ALLMOD	VALUE OF J (INDEX FOR Y LOCATION) WHEN SOLVING Z DIRECTION RADIATION FLUX.
JREF	MAIN	J LOCATION OF REFERENCE PRESSURE NODE.
JS	ALL	LOCAL VALUE OF JWLI+1.
JSTR	STRAD SOLVE STRIDF	STARTING J VALUE.
JSTR1	SOLVE STRAD	=JS-1.
JSUM	SOLVF	=JSTR+M.
JSUN	STRAD	=JS+JE.
JSUM	FPRINT	=JONE+MP1.
JSUM1	SOLVE	=JS+JE.
JSWP	SOLVE STRIDE	INDEX USED FOR X-TOMA SWEEP DIRECTION.
JSW1	INIT,MAIN ALLMOD	J NODE AT START OF DOME INLET.
JSW2	INIT,MAIN ALLMOD	J NODE AT END OF DOME INLET.
JTRAD	MAIN	TEMPORARY USAGE.
JU	SPRAY	=JUNIJ.
JUINJ	INIT,MAIN ALLMOD	J NODE LOCATIONS OF COOLING SLOTS.
JVINJ	INIT,MAIN ALLMOD	J NODE LOCATIONS OF RADIAL INJECTION HOLES.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
JWII	INIT,MAIN	J NODE AT WHICH UPSTREAM INNER INCLINED WALL STARTS.
JWIO	INIT,MAIN	J NODE AT WHICH UPSTREAM OUTER INCLINED WALL STARTS.
JWLI	ALL	STARTING J NODES OF THE CALCULATION DOMAIN AT INNER INCLINED WALL.
JWLO	ALL	ENDING J NODES OF THE CALCULATION DOMAIN AT OUTER INCLINED WALL.
JWOI	INIT,MAIN ALLMOD AUX STRIDE	J NODE AT WHICH DOWNSTREAM INNER INCLINED WALL ENDS.
JWOO	INIT,MAIN ALLMOD AUX STRIDE	J NODE AT WHICH DOWNSTREAM OUTER INCLINED WALL ENDS.
J1,J2	INIT	TEMPORARY VALUES FOR JWLI AND JWLO.
KEND	SOLVE	VALUE OF K AT LAST Z LOCATION.
KENDM1	SOLVE	=KEND-1.
KENDM2	SOLVE	=KEND-2.
KJC	SPRAY	TEMPORARY USAGE.
KJK	ALLMOD OUTPUT	TEMPORARY USAGE.
KJM	ALL	=KM(K)+JM(J).
KK	STRAD	TEMPORARY USAGE.
KLOC	SPRAY	K LOCATION OF DROPLET.
KM	ALL	=(K-1)*NJ*NK.
KMAX	MAIN ALLMOD	K LOCAION OF MAXIMUM CONTINUITY ERROR.
KMIN	SOLVE	=KSTR+1.
KOLD	SPRAY	PREVIOUS K LOCATION OF DROPLET.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
KONF	FPRINT	FIRST K VALUE FOR PRINTOUT.
KONTRO	AUX	CONTROL INDEX =1 ON FIRST ITERATION, OTHERWISE 2.
KONTRO	STRAD	CONTROL INDEX =1,2,3 WHEN NV=LVRX,LVRY,LVRZ.
KOUNT	TSOLVE	NUMBER OF ITERATIONS ON WALL TEMPERATURE.
KREF	MAIN	K LOCATION OF REFERENCE PRESSURE NODE.
KSTR	STRIDE STRAD AUX SOLVE	FIRST K LOCATION.
KSUM	SOLVE	=KEND+KSTR-2.
KSUM	STRAD	=2+N.
KVINJ	INIT ALLMOD MAIN	K NODE LOCATION OF RADIAL INJECTION HOLE.
L	ALL	=LP1-1.
LADIAB	CREK	SEE TABLE C-2.
LASTEP	MAIN STRIDE	MAXIMUM NUMBER OF ITERATIONS.
LCONVG	CREK	SEE TABLE C-2.
LCV	STRIDE	NUMBER OF CONTROL VOLUMES IN X DIRECTION(=L-1).
LDEBUG	CREK	SEE TABLE C-2.
LENER	CREK	=.FALSE., ENERGY EQUATION COMPLETELY DECOUPLED FROM SPECIES EQUATIONS AND SPECIES CONCENTRATIONS OBTAINED AT SPECIFIED TEMPERATURE, =.TRUE., COMPLETE ENERGY EQUATION IS USED.
LEQUIL	CREK	SEE TABLE C-2.
LIJ	ALL	=I+JM(J).
LIJNV	SOLVE	INDEX FOR VALUE AT K=1 PLANE IN F ARRAY.
LIJ2	STRIDE	=LIJ+KM(2).

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
LIK	AUXRAD STRAD	=I+KM(K).
LMOP,LMP3	AUX	TEMPORARY USAGE OF LP TYPE OF INDEX.
LNRG	CREK	SEE TABLE C-2.
LOMP,LOPM	AUX	TEMPORARY USAGE OF LP TYPE OF INDEX.
LOPP	AUX	TEMPORARY USAGE OF LP TYPE OF INDEX.
LP	ALL	=I+JM(J)+KM(K).
LPA	STRIDE	INDEX TO REFER TO Z- LOCATION.
LPC	ALL	TEMPORARY USAGE.
LPCE	SOLVE	TEMPORARY USAGE.
LPCH	AUX AUXRAD STRIDE SPRAY	INDEX USED TO REFER TO INTERMEDIATE HYDROCARBON MASS FRACTION.
LPCH1	STRIDE	INDEX USED TO REFER TO INTERMEDIATE HYDROCARBON MASS FRACTION.
LPCO	AUX AUXRAD STRIDE SPRAY	INDEX USED TO REFER TO CO MASS FRACTION.
LPCO1	STRIDE	INDEX USED TO REFER TO CO MASS FRACTION.
LPCSTR	SOLVE	TEMPORARY USAGE.
LPD	AUX	INDEX USED TO REFER TO DISSIPATION RATE.
LPE	STRIDE	INDEX TO REFER TO X+ LOCATION.
LPF	SOLVE STRIDE STRAD	INDEX FOR REFERING TO VALUE IN F ARRAY.
LPF	FPRINT	DO-LOOP LIMIT FOR PRINTOUT.
LPFAV	AUX STRIDE	INDEX USED TO REFER TO AVERAGE RADIATION FLUX.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINETION
LPFU	AUX AUXRAD STRIDE SPRAY	INDEX USED TO REFER TO UNBURNT FUEL MASS FRACTION.
LPFUOX	AUX AUXRAD STRIDE SPRAY	INDEX USED TO REFER TO MIXTURE FRACTION.
LPFU1	STRIDE	INDEX USED TO REFER TO UNBURNT FUEL MASS FRACTION.
LPF1	SOLVE	=LPF+ISTR1.
LPH	AUX STRIDE	INDEX USED TO REFER TO ENTHALPY.
LPHP	AUX	INDEX USED TO REFER TO ENTHALPY.
LPH2	AUX AUXRAD STRIDE SPRAY	INDEX USED TO REFER TO H2 MASS FRACTION.
LPH21	STRIDE	INDEX USED TO REFER TO H2 MASS FRACTION.
LPK	AUX	INDEX USED TO REFER TO TURBULENCE ENERGY.
LPL	FPRINT	DO-LOOP LIMIT FOR PRINTOUT.
LPMO	AUX	TEMPORARY USAGE OF LP TYPE OF INDEX.
LPN	ALLMOD	TEMPORARY USAGE.
LPN	STRIDE	INDEX TO REFER TO Y+ LOCATION.
LPN	AUX	INDEX USED TO REFER TO SOOT NUCLEUS CONCENTRATION.
LPNP1	ALLMOD STRIDE	TEMPORARY USAGE.
LPOM,LPOP	AUX	TEMPORARY USAGE OF LP TYPE OF INDEX.
LPO2	STRIDE	INDEX USED TO REFER TO O2 MASS FRACTION.
LPPO	AUX	TEMPORARY USAGE OF LP TYPE OF INDEX.
LPREF	STRIDE MAIN	LOCATION OF REFERENCE PRESSURE NODE.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
LPRX	AUX AUXRAD STRIDE	INDEX USED TO REFER TO X DIRECTION RADIATION FLUX.
LPRY	AUX AUXRAD STRIDE	INDEX USED TO REFER TO Y DIRECTION RADIATION FLUX.
LPRZ	AUXRAD STRIDE	INDEX USED TO REFER TO Z DIRECTION RADIATION FLUX.
LPS	AUX	INDEX USED TO REFER TO SOOT CONCENTRATION.
LPS	STRIDE	INDEX TO REFER TO Y- LOCATION.
LPSTR	SOLVE	TEMPORARY USAGE.
LPS1	AUX	INDEX USED TO REFER TO SOOT CONCENTRATION OF SIZE 1.
LPS2	AUX	INDEX USED TO REFER TO SOOT CONCENTRATION OF SIZE 2.
LPT	STRIDE	INDEX TO REFER TO Z+ LOCATION.
LPTE	AUX AUXRAD SPRAY	INDEX USED TO REFER TO TEMPERATURE.
LPW	ALLMOD STRIDE	INDEX TO REFER TO X- LOCATION.
LP1	ALL	NUMBER OF GRID NODES IN AXIAL (X) DIRECTION.
LP11	STRIDE	TEMPORARY USAGE.
LP2	ALLMOD STRIDE	TEMPORARY USAGE.
LREACT	CREK	SEE TABLE C-2.
LVCH	DATA ALLMOD AUX STRIDE	INDEX FOR INTERMEDIATE HYDROCARBON MASS FRACTION.
LVCH1	DATA STRIDE	INDEX FOR INTERMEDIATE HYDROCARBON MASS FRACTION.
LVCO	DATA ALLMOD AUX STRIDE	INDEX FOR CO MASS FRACTION.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
LVCO1	DATA STRIDE	INDEX FOR CO MASS FRACTION.
LVCO2	DATA	INDEX FOR CO2 MASS FRACTION.
LVD	DATA ALLMOD AUX	INDEX FOR DISSIPATION RATE OF TURBULENCE.
LVFU	DATA ALLMOD AUX STRIDE	INDEX FOR UNBURNT FUEL MASS FRACTION.
LVFUOX	DATA ALLMOD AUX STRIDE	INDEX FOR MIXTURE FRACTION.
LVFU1	DATA STRIDE	INDEX FOR UNBURNT FUEL MASS FRACTION.
LVH	DATA ALLMOD AUX STRIDE	INDEX FOR ENTHALPY.
LVH1	DATA ALLMOD AUX STRIDE	INDEX FOR H ATOM MASS FRACTION.
LVH2	DATA ALLMOD AUX STRIDE	INDEX FOR H2 MASS FRACTION.
LVH2O	DATA	INDEX FOR H2O MASS FRACTION.
LVH21	DATA STRIDE	INDEX FOR H2 MASS FRACTION.
LVK	DATA ALLMOD AUX STRIDE	INDEX FOR TURBULENCE KINETIC ENERGY.
LVN	DATA ALLMOD AUX	INDEX FOR SOOT NUCLEUS CONCENTRATION.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
LVNO	DATA	INDEX FOR NO MASS FRACTION.
LVNO2	DATA	INDEX FOR NO2 MASS FRACTION.
LVN1	DATA	INDEX FOR N ATOM MASS FRACTION.
LVN2	DATA	INDEX FOR N2 MASS FRACTION.
LVO	DATA	INDEX FOR O ATOM MASS FRACTION.
LVOH	DATA STRIDE	INDEX FOR OH MASS FRACTION.
LVO2	DATA STRIDE	INDEX FOR O2 MASS FRACTION.
LVRX	DATA ALLMOD STRIDE	INDEX FOR X DIRECTION RADIATION FLUX.
LVRY	DATA ALLMOD	INDEX FOR Y DIRECTION RADIATION FLUX.
LVRZ	DATA STRIDE	INDEX FOR Z DIRECTION RADIATION FLUX.
LVS1	DATA ALLMOD AUX	INDEX FOR MASS FRACTION OF SOOT PARTICLE SIZE 1.
LVS2	DATA ALLMOD AUX	INDEX FOR MASS FRACTION OF SOOT PARTICLE SIZE 2.
LXM	ALL	INDEX TO REFER TO X- LOCATION.
LXMC	ALLMOD SPRAY	TEMPORARY USAGE.
LXM1	AUX STRIDE	=LXM-NI.
LXP	ALL	INDEX TO REFER TO X+ LOCATION.
LXP1	AUX STRIDE	=LXP-NI.
LYM	ALL	INDEX TO REFER TO Y- LOCATION.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
LYMC	ALLMOD SPRAY	TEMPORARY USAGE.
LYM1	AUX	=LYM-1.
LYP	ALL	INDEX TO REFER TO Y+ LOCATION.
LYP1	AUX STRIDE	=LYP-1.
LZM	ALL	INDEX TO REFER TO Z- LOCATION.
LZMC	ALLMOD SPRAY	TEMPORARY USAGE.
LZM1	AUX	=LZM-1.
LZP	ALL	INDEX TO REFER TO Z+ LOCATION.
LZP1	AUX STRIDE	=LZP-1.
M	ALL	=MP1-1.
MAX	AUX STRIDE	LOCAL VALUE OF JWLO-1.
MCV	STRIDE	NUMBER OF CONTROL VOLUMES IN Y DIRECTION.
MIN	AUX	LOCAL VALUE OF JWLI+1.
MM1	STRIDE	SAME AS MCV.
MM1	ALLMOD	TEMPORARY USAGE.
MODEL	AUX,MAIN	INDEX FOR TYPE OF VISCOSITY(SEE INPUT).
MODEN	AUX,MAIN	INDEX FOR TYPE OF DENSITY(SEE INPUT).
MODER	AUX,MAIN STRIDE	INDEX FOR TYPE OF REACTION RATE(SEE INPUT).
MPART	AUX,MAIN	NUMBER OF SOOT PARTICLE SIZES.
MP1	ALL	NUMBER OF GRID NODES IN RADIAL (Y) DIRECTION.
MW	SPRAY	ARRAY TO STORE MOLECULAR WEIGHTS OF VARIOUS FUELS.
MWCOND	SPRAY	CONSTANT USED IN MOLECULAR WEIGHT CALCULATION.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
MWT	SPRAY	MOLECULAR WEIGHT OF FUEL VAPORS.
M1,M2	ALLMOD	TEMPORARY USAGE.
N	ALL	=NP1-1.
NA	CREK	SEE TABLE C-2.
NCV	STRIDE	NUMBER OF CONTROL VOLUMES IN Z DIRECTION(=N-1).
NDEBUG	CREK	SEE TABLE C-2.
NFNZ	SPRAY MAIN ALLMOD STRIDE INIT	INDEX FOR WHETHER LIQUID FUEL NOZZLE IS PRESENT (SEE INPUT).
NG	SPRAY	NUMBER OF DROPLET SIZE GROUPS.
NGAM	DATA STRIDE AUX	INDEX FOR DIFFUSION COEFFICIENT.
NGLOB	CREK	SEE TABLE C-2.
NGLOBP	CREK	SEE TABLE C-2.
NGOTO	STRIDE SOLVE STRAD ALLMOD AUX	INDEX WHICH TAKES VALUES 1,2,3 WHEN U,V,W BEING SOLVED, OTHERWISE IT HAS A VALUE OF 4.
NI	ALL	MAXIMUM NUMBER OF NODES IN X DIRECTION.
NINJ	STRIDE	NI*NJ.
NINJNK	STRIDE	NI*NJ*NK.
NITER	STRIDE	MAXIMUM NUMBER OF CHEMICAL KINETICS ITERATIONS.
NJ	ALL	MAXIMUM NUMBER OF NODES IN Y DIRECTION.
NK	ALL	MAXIMUM NUMBER OF NODES IN Z DIRECTION.
NLM	CREK	SEE TABLE C-2.
NN	SPRAY	DO-LOOP INDEX OVER FUEL NOZZLES.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
NNOX	MAIN	INDEX FOR NOX SOLUTION(SEE INPUT).
NNV	DATA STRIDE	MAXIMUM NUMBER OF DEPENDENT VARIABLES.
NP	DATA STRIDE	INDEX FOR PRESSURE.
NP1	ALL	NUMBER OF GRID NODES IN TANGENTIAL (Z) DIRECTION.
NQ	CREK	SEE TABLE C-2.
NRHO	DATA AUX	INDEX FOR DENSITY.
NS	ALL	NUMBER OF SPECIES.
NSKIP	FPRINT	TEMPORARY STORAGE FOR IPRINT.
NSL	SPRAY MAIN	NUMBER OF SPRAY CONE RAYS.
NSL2	SPRAY	=NSL(NN).
NSM	CREK	SEE TABLE C-2.
NSOOT	MAIN	INDEX FOR SOOT SOLUTION(SEE INPUT).
NS1,NS2	ALL	TEMPORARY USAGE OF DO-LOOP LIMITS ON SPECIES CONCENTRATIONS.
NTP	OUTPUT	INDEX FOR TAPE NUMBER.
NTPT	STRIDE	=NTP1+NTP2.
NTP1	STRIDE MAIN,INIT AUX	INDEX FOR TAPE NUMBER.
NTP2	STRIDE MAIN,INIT	INDEX FOR TAPE NUMBER.
NTPJ	SPRAY MAIN ALLMOD	INDEX FOR TAPE NUMBER.
NUINJ	MAIN,INIT ALLMOD	NUMBER OF COOLING SLOTS.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
NV	ALL	DEPENDENT VARIABLE INDEX.
NVCH	DATA,INIT ALLMOD STRIDE AUX	INDEX FOR INTERMEDIATE HYDROCARBON MASS FRACTION.
NVCO	DATA,INIT STRIDE AUX	INDEX FOR CO MASS FRACTION.
NVCO2	DATA	INDEX FOR CO2 MASS FRACTION.
NVD	DATA,INIT AUX	INDEX FOR DISSIPATION RATE OF TURBULENCE.
NVE		INDEX FOR EMISSIVE POWER.
NVF	ALL	INDEX FOR IDENTIFYING LOCATION IN F ARRAY.
NVFAV	DATA,INIT STRIDE AUX	INDEX FOR AVERAGE RADIATION FLUX.
NVFF	ALLMOD	=NVF(NV).
NVFU	DATA,INIT ALLMOD AUX STRIDE	INDEX FOR UNBURNT FUEL MASS FRACTION.
NVFUCX	DATA,INIT ALLMOD STRIDE AUX	INDEX FOR MIXTURE FRACTION.
NVH	DATA,INIT STRIDE AUX	INDEX FOR ENTHALPY.
NVHP	AUX	INDEX FOR ENTHALPY.
NVH2	DATA,INIT STRIDE AUX	INDEX FOR H2 MASS FRACTION.
NVH2O	DATA	INDEX FOR H2O MASS FRACTION.
NVINJ	MAIN INIT ALLMOD	NUMBER OF RADIAL INJECTION HOLES.

TABLE C-1 (CONT'D.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
NVJM	STRAD	=JM(J)+NVM(NVRZ).
NVK	DATA, INIT ALLMOD AUX	INDEX FOR TURBULENCE KINETIC ENERGY.
NVKM	SOLVE STRAD FPRINT	=KM(K)+NVM(NVF(NV)).
NVM	ALL	=(NV-1)*NI*NJ*NK.
NVN	DATA, INIT AUX	INDEX FOR SOOT NUCLEUS CONCENTRATION.
NVN2	DATA	INDEX FOR N2 MASS FRACTION.
NVOX	DATA	INDEX FOR O2 MASS FRACTION.
NVRX	DATA, INIT STRIDE	INDEX FOR X DIRECTION RADIATION FLUX.
NVRY	DATA, INIT STRIDE	INDEX FOR Y DIRECTION RADIATION FLUX.
NVRZ	DATA, INIT STRIDE ALLMOD	INDEX FOR Z DIRECTION RADIATION FLUX.
NVS1	DATA, INIT AUX	INDEX FOR MASS FRACTION OF SOOT PARTICLE SIZE 1.
NVS2	DATA, INIT AUX	INDEX FOR MASS FRACTION OF SOOT PARTICLE SIZE 2.
NVTF	DATA, INIT AUX	INDEX FOR TEMPERATURE.
NVV	FPRINT	DO-LOOP COUNTER.
NVVV	FPRINT	FIRST DEPENDENT VARIABLE TO BE PRINTED ON A CALL TO FPRINT.
N1	CREK	SEE TABLE C-2.
N2	CREK	SEE TABLE C-2.
N3	CREK	SEE TABLE C-2.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
OGPSI	AUX	TEMPORARY USAGE.
OGPSIR	AUX	TEMPORARY USAGE.
P	ALL	PRESSURE.
PA	CREK	PRESSURE.
PATH	AUXRAD	PATH LENGTH FOR RADIATION CALCULATIONS.
PRAR	OUTPUT	TEMPORARY USAGE.
PCO2	AUXRAD	CO2 PARTIAL PRESSURE.
PEXP1	INIT	PRE-EXPONENT FACTOR IN FIRST STEP OF HYDROCARBON OXIDATION SCHEME.I
PEXP2	INIT	PRE-EXPONENT FACTOR IN SECOND STEP OF HYDROCARBON OXIDATION SCHEME.
PEXP3	INIT	PRE-EXPONENT FACTOR IN THIRD STEP OF HYDROCARBON OXIDATION SCHEME.
PEXP4	INIT	PRE-EXPONENT FACTOR IN FOURTH STEP OF HYDROCARBON OXIDATION SCHEME.I
PHI	INIT AUX	FUEL MASS FRACTION/STOICHIOMETRIC MIXTURE FRACTION.
PH2O	AUXRAD	H2O PARTIAL PRESSURE.
PI	SPRAY	=3.14159.
PJAY	ALLMOD MAIN	PJAY FUNCTION FOR HEAT TRANSFER WALL FUNCTION.
PLAXM1	ALL	IPLAX-1.
PLPREF	STRIDE	PRESSURE AT REFERENCE PRESSURE LOCATION.
PO,POT	SPRAY	CONSTANTS IN BOILING POINT CALCULATION.
PO2	AUX	OXYGEN PARTIAL PRESSURE.
PP	ALL	PRESSURE CORRECTION.
PPLN	CREK	SEE TABLE C-2.
PR	AUX, MAIN ALLMOD	LAMINAR PRANDTL/SCHMIDT NUMBER.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
PRFF	AUX,MAIN ALLMOD	TURBULENT PRANDTL/SCHMIDT NUMBER.
PRESS	MAIN INIT STRIDE AUX	SYSTEM PRESSURE.
PREXPS	AUX,MAIN	PRE-EXPONENT FACTOR IN SOOT OXIDATION RATE (SEE INPUT).
PREXP1	AUX,MAIN INIT	PRE-EXPONENT FACTOR IN FIRST STEP OF HYDROCARBON OXIDATION SCHEME(=PEXP1).
PREXP2	AUX,MAIN INIT	PRE-EXPONENT FACTOR IN SECOND STEP OF HYDROCARBON OXIDATION SCHEME(=PEXP2).
PREXP3	AUX,MAIN INIT	PRE-EXPONENT FACTOR IN THIRD STEP OF HYDROCARBON OXIDATION SCHEME(=PEXP3).
PREXP4	AUX,MAIN INIT	PRE-EXPONENT FACTOR IN FOURTH STEP OF HYDROCARBON OXIDATION SCHEME(=PEXP4).
PRRAT	MAIN	RATIO OF LAMINAR AND TURBULENT PRANDTL NUMBERS.
PR3	SPRAY	PRANDTL NUMBER.
PSI	AUX	FRACTION OF FINE STRUCTURES HEATED ENOUGH TO REACT.
PSIC	AUX	TEMPORARY USAGE IN SOOT OXIDATION RATE.
PT2	SPRAY	=2*PI.
QCH	TSOLVE	CONVECTION HEAT TRANSFER.
QDOT	SPRAY	HEAT TRANSFER RATE TO DROPLET.
QRH	TSOLVE	NET RADIATION HEAT TRANSFER FROM WALL.
Q0-Q4	CREK	SEE TABLE C-2.
R	ALL	RADIUS.
RAD	TSOLVE	RADIATION HEAT FLUX TO WALL.
RADIN	INIT ALLMOD	INLET RADIATION FLUX.
RADSUR	INIT ALLMOD	RADIATION FLUX AT EACH AXIAL STATION.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
RATE	SPRAY	DROPLET EVAPURATION RATE.
RATIO1-9	INIT ALLMOD AUX	CONSTANTS USED IN ELEMENT BALANCE EQUATIONS.
RATO10-12	INIT ALLMOD AUX	CONSTANTS USED IN ELEMENT BALANCE EQUATIONS.
RDT	STRIDE	ALWAYS EQUAL TO ZERO.
REI	SPRAY	DROPLET REYNOLDS NUMBER.
RELAX	SOLVE MAIN STRIDE AUX	UNDER-RELAXATION FACTORS (SEE INPUT).
RELAXM	SOLVE AUX	=1.-RELAX.
RET	AUX	TURBULENT REYNOLDS NUMBER.
RFUEL	MAIN SPRAY	RADIUS OF FUEL NOZZLE.
RF1,RF2	AUX	SOOT FORMATION RATES.
RGAS	CREK	SEE TABLE C-2.
RGASIN	CREK	SEE TABLE C-2.
RHO	ALL	DENSITY.
RHOA	ALLMOD STRIDE	DENSITY*AREA.
RHOCON	MAIN AUX	PRESSURE DIVIDED BY UNIVERSAL GAS CONSTANT.
RHOINJ	ALLMOD	DENSITY OF DILUTION JET.
RHOLP	AUX	DENSITY AT NODE LP.
RHOO	AUX	DENSITY OF SURROUNDING FLUID.
RHOP	AUX MAIN INIT	SOOT PARTICLE DENSITY.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
RHOPP	STRIDE INIT	DENSITY AT NODE P.
RHOSTR	AUX	DENSITY OF FINE STRUCTURES.
RHOSW	INIT ALLMOD	INLET DENSITY.
RHO4	INIT	DENSITY.
RI	STRIDE MAIN	INNER RADIUS OF COMBUSTOR.
RM	STRIDE	RADIUS AT V-VELOCITY LOCATION.
RMV	STRIDE	RADIUS AT V-VELOCITY CONTROL VOLUME SURFACE.
RNC	AUX	TEMPORARY USAGE.
RNG	SPRAY	NUMBER OF DROPLET SIZE GROUPS.
RNSL	SPRAY MAIN INIT	=NSL2, NUMBER OF SPRAY CONE RAYS.
ROA	ALLMOD	DENSITY*AREA.
ROF	SPRAY	DENSITY OF LIQUID FUEL AT BOILING POINT.
ROFO	SPRAY	INITIAL DENSITY OF LIQUID FUEL.
ROST	SPRAY	GAS DENSITY.
RTCD	INIT ALLMOD AUX	SQUARE ROOT OF CD.
RTCDK	ALLMOD	TURBULENCE ENERGY*SQRT(CD).
RVAV	STRIDE	TEMPORARY USAGE.
RVECX-Z	SPRAY	COORDINATE TRANSFORMATION QUANTITIES.
SBAR	OUTPUT	TEMPORARY USAGE.
SCATR	AUXRAD MAIN INIT	SCATTERING COEFFICIENT (IF ITRAD=2).

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
SCTR	AUXRAD	ARRAY FOR SCATTERING COEFFICIENT.
SC3	SPRAY	SCHMIDT NUMBER.
SECTOR	INIT	ANGULAR SECTOR.
SEXIT	ALLMOD	EXIT MASS FLOW ERROR.
SFAC	AUX	TEMPORARY USAGE IN CO REACTION RATE.
SHRSTR	ALLMOD	SHEAR STRESS.
SIG	TSOLVE	STEFAN-BOLTZMANN CONSTANT.
SIGMA	AUXRAD DATA ALLMOD INIT AUX	STEFAN-BOLTZMANN CONSTANT.
SINA	SPRAY	SINE OF HALF THE NOZZLE CONE ANGLE.
SINB	SPRAY	SINE OF NOZZLE BACK ANGLE.
SIND	SPRAY	SINE OF NOZZLE DOWN ANGLE.
SINT	SPRAY	SINE OF CURRENT SPRAY CONE SEGMENT ANGLE.
SKE	ALLMOD	TURBULENCE ENERGY AT COOLING SLOT.
SLM	ALLMOD	LENGTH SCALE AT COOLING SLOT.
SM	CREK	SEE TABLE C-2.
SMASS	INIT	TEMPORARY USAGE.
SMAX	ALLMOD MAIN	MAXIMUM OF CONTINUITY ERRORS.
SMCONC	OUTPUT	SMOKE CONCENTRATION.
SMD	SPRAY MAIN	SAUTER MEAN DIAMETER.
SMINV	CREK	SEE TABLE C-2.
SMONO	OUTPUT	SMOKE NUMBER.
SMW	CREK	SEE TABLE C-2.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
SMO	CREK	NOT USED.
SNOX	MAIN	NOX SOLUTION STARTED AFTER ERROR FALLS TO SNOX OR AFTER INOX NUMBER OF ITERATIONS.
SOOTK	AUXRAD	SOOT CONCENTRATION.
SOOT1	ALL	MASS FRACTION OF SOOT PARTICLE SIZE 1.
SOOT2	ALL	MASS FRACTION OF SOOT PARTICLE SIZE 2.
SOR	AUX	PART OF SOURCE TERM.
SORCO	AUX	PART OF CO SOURCE TERM.
SOR1	AUX	LAMINAR SOURCE TERM.
SOR2	AUX	TURBULENT SOURCE TERM.
SOR3	AUX	LAMINAR SOURCE TERM.
SOR4	AUX	TURBULENT SOURCE TERM.
SP	ALL	PART OF LINEARIZED SOURCE TERM.
SPCH	AUX	PART OF LINEARIZED SOURCE TERM (SP) FOR INTERMEDIATE HYDROCARBON MASS FRACTION.
SPC1,SPC2	AUX	SOOT OXIDATION RATE.
SPFU	AUX	PART OF LINEARIZED SOURCE TERM (SP) FOR FUEL.
SPF1,SPF2	AUX	TEMPORARY USAGE.
SPF2F	AUX	TEMPORARY USAGE.
SPK	SOLVE	PART OF LINEARIZED SOURCE TERM USED IN CYCLIC TDMA.
SQFK	INIT	SQUARE ROOT OF FK.
SRAD	MAIN	RADIATION SOLUTION STARTED AFTER ERROR FALLS TO SRAD OR AFTER IRAD NUMBER OF ITERATIONS.
SREI	SPRAY	SQUARE ROOT OF REI.
SSOOT	MAIN	SOOT SOLUTION STARTED AFTER ERROR FALLS TO SSOOT OR AFTER ISOOT NUMBER OF ITERATIONS.
SSS	AUX	TEMPORARY USAGE.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
SSUM	ALLMOD MAIN	SUM OF ABSOLUTE CONTINUITY ERRORS.
STORE	SOLVE STRAD	TEMPORARY USAGE.
ST4	INIT	*SIGMA*TEMP**4.
SU	ALL	PART OF LINEARIZED SOURCE TERM.
SUCH	AUX	PART OF LINEARIZED SOURCE TERM (SU) FOR INTERMEDIATE HYDROCARBON MASS FRACTION.
SUFU	AUX	PART OF LINEARIZED SOURCE TERM (SU) FOR FUEL.
SUF1,SUF2	AUX	TEMPORARY USAGE.
SUK	SOLVE	PART OF LINEARIZED SOURCE TERM USED IN CYCLIC TDMA.
SUM	AUX	TEMPORARY USAGE.
SUM1	MAIN	TEMPORARY USAGE.
SUM2	MAIN	TEMPORARY USAGE.
SWNO	MAIN	RATIO OF TANGENTIAL TO AXIAL VELOCITY AT DOME INLET.
S1	CREK	SEE TABLE C-2.
S2	CREK	SEE TABLE C-2.
T	INIT AUXRAD AUX	TEMPERATURE.
TAN	INIT	ANNULUS TEMPERATURE.
TAUP	AUX	WALL SHEAR STRESS.
TB	SPRAY	LIQUID FUEL BOILING TEMPERATURE.
TCYLW	ALLMOD MAIN	TEMPERATURE OF CYLINDRICAL PORTION OF COMBUSTOR WALL.
TEMP	ALL	TEMPERATURE.
TEMPW	ALLMOD	TEMPERATURE.
TEMTM	INIT	MASS AVERAGED TEMPERATURE AT EACH AXIAL STATION.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
TF	SPRAY	TEMPERATURE OF COMBUSTION PRODUCTS.
TFU	SPRAY	LIQUID DROPLET TEMPERATURE.
TFUEL	MAIN ALLMOD SPRAY	INLET TEMPERATURE OF FUEL.
TGAS	TSOLVE	GAS TEMPERATURE.
THETA	SPRAY	CURRENT SPRAY CONE SEGMENT ANGLE.
THETA1	SPRAY MAIN	INITIAL SPRAY CONE SEGMENT ANGLE.
THETA2	SPRAY MAIN	FINAL SPRAY CONE SEGMENT ANGLE.
TIME	STRIDE	TIME.
TIN	INIT	INITIAL TEMPERATURE AT EACH AXIAL STATION.
TINCP	AUX MAIN	SOOT CALCULATION BYPASSED FOR TEMPERATURE.LE.TINCP.
TINLW	ALLMOD MAIN INIT	TEMPERATURE OF INCLINED WALL PORTION OF COMBUSTOR AND OF DOME.
TITLE	FPRINT MAIN	HEADING FOR DEPENDENT VARIABLE.
TITLE2	OUTPUT MAIN	CASE TITLE CARD.
TK	CREK	SEE TABLE C-2.
TKINV	CREK	SEE TABLE C-2.
TLIP	ALLMOD MAIN	TEMPERATURE OF COOLING SLOT LIP.
TLN	CREK	SEE TABLE C-2.
TMAX	INIT AUX	MAXIMUM TEMPERATURE.
TNEW	INIT	TEMPERATURE ON NEW ITERATION.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
TNOX	MAIN STRIDE	NOX CALCULATION BYPASSED IF TEMPERATURE.LE.TNOX.
TO	AUX	TEMPERATURE OF SURROUNDING FLUID.
TOUT		OUTLET TEMPERATURE (NOT USED).
TS	AUXRAD	TEMPERATURE.
TST	SPRAY	GAS TEMPERATURE.
TSTR	AUX	TEMPERATURE OF FINE STRUCTURES.
TSW	INIT MAIN	TEMPERATURE AT DOME INLET.
TWINJ	ALLMOD MAIN INIT	COOLING SLOT TEMPERATURE.
TVINJ	MAIN INIT	DILUTION JET TEMPERATURE.
TW	TSOLVE	WALL TEMPERATURE.
TWN	TSOLVE	WALL TEMPERATURE AT NEW ITERATION.
TW2	TSOLVE	=TW**2.
TX,TX1	STRIDE STRAD	DIFFUSION FLUX IN X DIRECTION.
TY,TY1	STRIDE STRAD	DIFFUSION FLUX IN Y DIRECTION.
TZ	STRIDE STRAD	DIFFUSION FLUX IN Z DIRECTION.
TZFAC	STRIDE	FRACTION OF DIFFUSION FLUX IN Z DIRECTION.
T1	SPRAY	AVERAGE OF TB AND TF.
T4	INIT	TEMPORARY USAGE.
U	ALL	U-VELOCITY.
UADD	ALLMOD	CORRECTION TO EXIT VELOCITIES.
UF	SPRAY	DROPLET VELOCITY IN X DIRECTION AT CURRENT LOCATION.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
UFO	SPRAY	DROPLET VELOCITY IN X DIRECTION AT PREVIOUS LOCATION.
UIN	INIT	MEAN U-VELOCITY AT EACH AXIAL STATION.
UINJ	ALLMOD MAIN INIT	COOLING SLOT AXIAL VELOCITY.
ULIM	SPRAY	LIMIT ON DROPLET VELOCITY CHANGE BETWEEN SUCCESSIVE STEPS.
UMASS	INIT	MOMENTUM FLOW THROUGH DOME INLET.
UMEAN	ALLMOD	MEAN EXIT VELOCITY.
UNICON	DATA ALLMOD STRIDE AUX INIT	UNIVERSAL GAS CONSTANT.
UST	SPRAY	GAS VELOCITY IN X DIRECTION.
USW	INIT MAIN	AXIAL VELOCITY OF DOME INLET.
UYM,UYP	AUX	AVERAGE U VELOCITY BETWEEN NEIGHBORING NODES.
UZM,UZP	AUX	AVERAGE U VELOCITY BETWEEN NEIGHBORING NODES.
V	ALL	V-VELOCITY.
VC,VEC	AUX	RESULTANT VELOCITY.
VECX-Z	SPRAY	UNIT VECTORS IN X,Y,Z DIRECTIONS.
VF	SPRAY	DROPLET VELOCITY IN Y DIRECTION AT CURRENT LOCATION.
VFO	SPRAY	DROPLET VELOCITY IN Y DIRECTION AT PREVIOUS LOCATION.
VFU	SPRAY	RESULTANT DROPLET VELOCITY AT CURRENT LOCATION.
VFUEL	SPRAY MAIN	INITIAL FUEL DROPLET VELOCITY.
VINJ	INIT ALLMOD MAIN	RADIAL VELOCITY OF DILUTION JET.
VISC	ALL	VISCOSITY.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
VISCO	SPRAY	GAS VISCOSITY.
VISCOS	AUX	VISCOSITY.
VMIX	AUX AUXRAD	RECIPROCAL OF AVERAGE MOLECULAR WEIGHT.
VMT2	AUX	AVERAGE V VELOCITY BETWEEN NEIGHBORING NODES.
VOL	STRIDE	VOLUME OF ELEMENTARY CONTROL VOLUME.
VP	AUX	RESULTANT VELOCITY.
VPT2	AUX	AVERAGE V VELOCITY BETWEEN NEIGHBORING NODES.
VR	SPRAY	RESULTANT RELATIVE VELOCITY BETWEEN GAS AND DROPLET.
VST	SPRAY	GAS VELOCITY IN Y DIRECTION.
VSW	INIT MAIN	RADIAL VELOCITY OF DOME INLET.
VXM,VXP	AUX	AVERAGE V VELOCITY BETWEEN NEIGHBORING NODES.
VZM,VZP	AUX	AVERAGE V VELOCITY BETWEEN NEIGHBORING NODES.
W	ALL	W-VELOCITY.
WALKE	ALLMOD	WALL TURBULENCE KINETIC ENERGY.
WCH	INIT AUX	MOLECULAR WEIGHT OF INTERMEDIATE HYDROCARBON.
WCO	INIT,DATA AUX	MOLECULAR WEIGHT OF CO.
WCO2	INIT,DATA AUX	MOLECULAR WEIGHT OF CO2.
WC2H4	INIT,DATA	MOLECULAR WEIGHT OF C2H4.
WF	SPRAY	DROPLET VELOCITY IN Z DIRECTION AT CURRENT LOCATION.
WFF	SPRAY MAIN INIT	FUEL FLOW RATE.
WFI	SPRAY	FUEL FLOW RATE ON A PARTICULAR RAY.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
WFN7	INIT	TOTAL LIQUID FUEL FLOW RATE.
WFO	SPRAY	DROPLET VELOCITY IN Z DIRECION AT PREVIOUS LOCATION.
WFU	INIT, DATA AUX	MOLECULAR WEIGHT OF FUEL.
WH2	INIT, DATA AUX	MOLECULAR WEIGHT OF H2.
WH20	INIT, DATA AUX	MOLECULAR WEIGHT OF H20.
WIN	ALLMOD	W-VELOCITY THROUGH DOME INLET.
WL7P	STRIDE	TEMPORARY USAGE.
WMNM, WMNP	AUX	AVERAGE W VELOCITY BETWEEN NEIGHBORING NODES.
WN2	INIT, DATA AUX	MOLECULAR WEIGHT OF N2.
WOX	INIT, DATA AUX	MOLECULAR WEIGHT OF 02.
WST	SPRAY	GAS VELOCITY IN Z DIRECTION.
WSW	INIT ALLMOD	TANGENTIAL VELOCITY OF DOME INLET.
WUINJ	ALLMOD MAIN INIT	COOLING SLOT TANGENTIAL VELOCITY.
WXM, WXP	AUX	AVERAGE W VELOCITY BETWEEN NEIGHBORING NODES.
WYM, WYP	AUX	AVERAGE W VELOCITY BETWEEN NEIGHBORING NODES.
X	ALL	AXIAL DISTANCE.
XDIF	STRIDE	INTERNODAL DISTANCE IN X-DIRECTION.
XF	SPRAY	X LOCATION OF DROPLET.
XM	SPRAY	X LOCATION OF CONTROL VOLUME SURFACES.
XM	AUX	X DISTANCE AT X- LOCATION.
XO	MAIN SPRAY	X LOCATION OF ORIGIN OF FUEL NOZZLE SPRAY.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINITION
XP	AUX	X DISTANCE AT X+ LOCATION.
XS	STRIDE	MAIN CONTROL VOLUME WIDTH IN X DIRECTION.
XSU	STRIDE	U-VELOCITY CONTROL VOLUME WIDTH IN X DIRECTION.
Y	ALL	RADIAL DISTANCE.
YDIF	STRIDE	INTERNODAL DISTANCE IN Y DIRECTION.
YF	SPRAY	Y LOCATION OF DROPLET.
YM	SPRAY	Y LOCATION OF CONTROL VOLUME SURFACES.
YM	AUX	Y DISTANCE AT Y- LOCATION.
YO	MAIN SPRAY	Y LOCATION OF ORIGIN OF FUEL NOZZLE SPRAY.
YP	AUX	Y DISTANCE AT Y+ LOCATION.
YPLUS	ALLMOD	YPLUS IN WALL FUNCTIONS.
YS	STRIDE	MAIN CONTROL VOLUME WIDTH IN Y DIRECTION.
YSR	STRIDE	MAIN CONTROL VOLUME AREA NORMAL TO X DIRECTION.
YSV	STRIDE	V-VELOCITY CONTROL VOLUME WIDTH IN Y DIRECTION.
YSVR	STRIDE	V-VELOCITY CONTROL VOLUME AREA NORMAL TO X DIRECTION.
Y1,Y2	INIT	TEMPORARY USAGE.
Z	ALL	TANGENTIAL DISTANCE.
ZDIF	STRIDE	INTERNODAL DISTANCE IN Z DIRECTION.
ZF	SPRAY	Z LOCATION OF DROPLET.
ZM	SPRAY	Z LOCATION OF CONTROL VOLUME SURFACES.
ZM	AUX	Z DISTANCE AT Z- LOCATION.
ZO	MAIN SPRAY	Z LOCATION OF ORIGIN OF FUEL NOZZLE SPRAY.
ZP	AUX	Z DISTANCE AT Z+ LOCATION.
ZS	STRIDE	MAIN CONTROL VOLUME WIDTH IN Z DIRECION.

TABLE C-1 (CONTD.)

FORTRAN VARIABLE	SUBROUTINE WHERE DEFINED OR USED OFTEN	DEFINETION
ZSMALL	SPRAY	ONE HUNDRETH OF AVERAGE ANGULAR GRID SPACING.
ZSW	STRIDE	W-VELOCITY CONTROL VOLUME WIDTH IN Z DIRECTION.

TABLE C-2. LIST OF FORTRAN VARIABLES IN THE CHEMICAL KINETICS PROGRAM CREK.

This list is adapted from Ref. 48 to which the reader is referred for further details.

Fortran Variable	Routines Where Defined Or Used Often	Definition
A	CALC	Elements of Newton-Raphson correction matrix.
AL	CREKO SPECE CALC	Atomic stoichiometric coefficients, AL(I,J) = the number of kg-atoms of element I per kg-mole of species J.
ATOM	ERATIO (SPECE) CREKO	ATOM (1,K) = atomic symbol for element K. ATOM (2,K) = atomic weight of element K. ATOM (3,K) = valence or oxidation state of element K.
ASUB	CREKO	Molecular symbol of each NS species (e.g., CO, H_2O, etc.).
BO	SPECE CALC	Atom numbers for reactant mixture, BO(I) = kg-atoms element I per kg reactant mixture.
BX	CREKO CALC	Exponent-on 10 on pre-exponential term of extended Arrhenius forward rate expression, when read from MECHANISM data cards. Later, BX is set = BX*($\log_e$10) to avoid repetitive exponentiation on ten.
BX2	CREKO CALC	Same as BX for reverse rate expression.
CPSUM	CALC CREKO HCPS	Non-dimensional mixture constant pressure specific heat capacity.
EMV	CREK CALC	Total convective and diffusive mass inflow rate to the control volume, kg m^{-3} s^{-1}.
ER	CREK ERATIO (SPECE)	Fuel/air equivalence ratio.

TABLE C-2 (Continued).

Fortran Variable	Routines Where Defined Or Used Often	Definition
ETA	SPECE	Self-adjusting under-relaxation parameter.
FQ	CREK CALC	Scaling parameter for Q.
HO	CREKO CALC HCPS	Non-dimensional, ideal-gas enthalpy of each chemical species at given temperature.
HSUBO	CREKO CALC	Convective and diffusive net enthalpy influx rate to the control volume, divided by EMV (i.e., mass-averaged specific enthalpy of reactants entering the control volume), J/kg. HSUBO must be set by the calling program.
HSUM	CREKO CALC	Working variable wherever used.
ID	CREKO CALC	ID(K,J) is the species index number (i=1, NS) of the K-th species (K=1,4) in the J-th reaction (J=1,JJ).
IDCO, IDC02 IDH2, IDH20 IDN2, ID02	CALC	Index number (i=1,NS) of the particular species in the variable name.
IHCPS	CREKO CALC HCPS	Value of IHCPS controls whether or not subroutine HCPS calculates values of non-dimensional one-atmosphere entropy for each species.
ILC, ILH	CREKO CALC	Index number of the elements carbon and hydrogen, respectively.
IMAT	SPECE CALC	Number of rows in Newton-Raphson correction matrix; set in CALC. IMAT=N2 if LEQUIL=.TURE.: IMAT=NQ if LEQUIL=.FALSE.

TABLE C-2 (Continued)

Fortran Variable	Routines Where Defined Or Used Often	Definition
ITER	SPECE	Current value of iteration counter.
ITMAX	SPECE	Controls the maximum number of iterations permitted by each call to CREK. Set by DATA statement in SPECE.
JJ	CREKO CALC	Number of distinct forward reactions considered in reaction mechanism; must be less than or equal to the dimensions of labeled COMMON block REACTS.
LADIAB	CREK CALC	LADIAB must be set by program calling CREK. If =.FALSE., enthalpy source term Q is non-zero, and calling program must specify values of Q0, Q1, Q2, Q3 and Q4 in enthalpy source term.
LCONVG	CREK SPECE	Initially = .FALSE.; set = .TRUE. in SPECE if convergent solution achieved. Controls solution strategy in CREK.
LDEBUG	SPECE CALC	If LDEBUG is set = .TRUE. by the calling program, intermediate output is written on the output record. Default value is .FALSE.
LEQUIL	CREK SPECE CALC	LEQUIL must be set by calling program. If = .TRUE., equilibrium states are calculated; if = .FALSE., kinetic stationary states are calculated.
LNRG	CREK CALC	For LEQUIL = .FALSE. problems only. If = .TRUE., fully coupled energy equation is used.
LREACT	CREK	LREACT = .FALSE. on entry to CREK suppresses calculation of combustion reaction. Default value is .TRUE.

TABLE C-2 (Continued)

Fortran Variable	Routines Where Defined Or Used Often	Definition
NDEBUG	CREK SPECE CALC	When LDEBUG = .TRUE., NDEBUG set from 1 to 5 controls increasing detail of debug output. Default value of NDEBUG = 5.
NGLOB	CREKO CALC	Number of finite-rate global hydrocarbon pyrolysis steps considered.
NGLOBP	CREKO CALC	NGLOB + 1.
NLM	CREKO SPECE CALC	The number of distinct elements considered. Must be less than or equal to corresponding dimensions of labeled COMMON block CEQUIL.
N1,N2,N3	CREKO CALC	N1 = NLM + 1, N2 = NLM + 2, N3 = NLM + 3.
NS	CREKO SPECE CALC	Number of distinct speces considered. Must be less than appropriate dimensions in labeled COMMON blocks CEQUIL, CMATRI, CPARAM and CSPECE.
NSM, NQ, NA	CREKO CALC	NSM = NS +1, NQ = NS + 2, NA = NS + 3.
PA	CREK SPECE CALC	Pressure within control volume, N m^{-2}. Must be set by program calling CREK.
PI	CALC	Lagrange multipliers in reduced Gibbs iteration correction equatations.
PPLN	CREK CALC	$\text{Log}_e\ (P/P_o)$.
Q	CALC	Negative of non-dimensional enthalpy source term, determined by values of Q0, Q1, Q2, Q3 and Q4 set by the calling program.

TABLE C-2 (Continued)

Fortran Variable	Routines Where Defined Or Used Often	Definition
Q0, Q1, Q2, Q3, Q4	CALC	Coefficients for enthalpy source term, $-S_H = Q_0 + QT + Q_2T^2 + Q_3T^3 + Q_4T^4$, $Jm^{-3}\ s^{-1}$. These values must be set whenever LADIAB = .FALSE. is set by the calling program.
RGAS	CREKO CALC	Universal gas constant, 8314.4 J/(kg-mole)(K).
RGASIN	CREKO CALC	Inverse of RGAS.
RHOP	CREKO CALC	Mass density , kg m^{-3}.
RT	CALC	$\frac{\partial f_i}{\partial \log T}$
SO	CREKO CALC HCPS	One-atmosphere, ideal-gas entropy of species i.
S1	CREKO CALC	Inlet mole numbers of species i.
S2	CREKO CALC	Mole numbers of species i, kg-moles i/kg. Calling program must set these values as estimates; on return they are solution values.
SM	ALL	Reciprocal mixture molecular weight.
SMINV	CREK CALC	Reciprocal of SM, therefore the mixture molecular weight, kg/(kg-mole).
SMW	CREKO	Molecular weight of species i.
SSAVE	CREK	Array for saving current values of S2.

TABLE C-2 (Continued)

Fortran Variable	Routines Where Defined Or Used Often	Definition
TACT, TACT2	CREKO CALC	Activation temperature (activation energy divided by gas constant) for forward and reverse reactions respectively, degrees K.
TEN, TEN2	CREKO CALC	Exponent-on-temperature in pre-exponential term of rate constant in forward and reverse reactions respectively.
TK	ALL	Temperature T, deg K. Estimate on calling CREK, solution on return. If set equal to zero by program calling CREK, causes CREK to establish estimates for T and S2.
TKINV	CREK CALC	Reciprocal of TK.
TLN	CREKO CALC HCPS	Logarithm of the temperature.
X	CREKO CALC	Current values of the correction variables: Also used as working variable in subroutine CREKO.
X1, X2	CALC	Contact index for forward and reverse reactions j. Dimensionless.
Y	CREKO CALC	Logarithms of variables. Also used as working variable in subroutine CREKO.
Z	CREKO HCPS	Coefficients for calculation of thermochemical data.

APPENDIX D

LISTING OF THE 3-D COMBUSTOR PERFORMANCE PROGRAM

APPENDIX D

LISTING OF THE 3-D COMBUSTOR PERFORMANCE PROGRAM

This appendix contains a listing of the 3-D combustor performance program. In order to identify the changes made to the original program of Ref. 1, various correction idents appear at the ends of the changed or newly inserted statements. The meanings of these correction idents are given below:

CREK CALC SPEC CRKO HCPS	-	Chemical kinetics program CREK
ABSOR	-	Radiation-property subroutine
SOOT	-	Soot-emissions updates
NASAX	-	Corrections to the original program
CTDMA	-	Cyclic TDMA updates
NOXXX	-	Updates to make the chemical kinetics program CREK CYBER-Compatible
RAD TS0	-	Radiation updates
NOX	-	NO_x-emissions updates for 3-D program
NOXX	-	NO_x-emissions updates for CREK program
4STEP	-	4-Step-mechanism updates
COMMENT	-	Comment cards
JAN14 JAN18 FEB2 MAR2	-	Some additional modifications

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      PROGRAM MAIN(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE8,TAPE9,     NASAX     1
     1 TAPE11)                                                            NASAX     2
      COMMON F(500,7),DU(10,10,5),DV(10,10,5),DW(10,10,5),                COMFA     2
     1 ANUC(10,10,5),SQOT1(10,10,5),SQOT2(10,10,5),FCH(10,10,5),          4STEP     1
     2 FH2(10,10,5),FS(500,14),                                           4STEP     2
     1 RHO(10,10,5),VISC(10,10,5),ABSR(10,10,5),SCTR(10,10,5),            RAD       1
     1 SU(10,10),SP(10,10),DRHODP(10,10,5),                               RAD       2
     1  AXP(10,10),AXM(10,10),AYP(10,10),AYM(10,10),AZP(10,10),           COMFA     4
     2  AZM(10,10),C7(10,10),CY(10),CZU(10,10),CYU(10),                   COMFA     5
     3  CZP(10,10),CYP(10),DIVG(10,10),NTP1,NTP2                          COMFA     6
     1,AXMK(192),AXPK(192),AYMK(192),AYPK(192),AZMK(192),AZPK(192),       CTDMA     1
     2 SUK(192),SPK(192)                                                  CTDMA     2
      DIMENSION U(10,10,5),V(10,10,5),W(10,10,5),PP(10,10,5)              COMFA     7
      DIMENSION P(10,10,5),TEMP(10,10,5),GAM(10,10,5)                     COMFA     8
      EQUIVALENCE (F(1,1),U(1,1,1)),(F(1,2),V(1,1,1)),(F(1,3),W(1,1,1))   COMFA     9
      EQUIVALENCE (F(1,4),PP(1,1,1)),(F(1,5),P(1,1,1))                    COMFA    10
      EQUIVALENCE (F(1,6),TEMP(1,1,1)),(F(1,7),GAM(1,1,1))                COMFA    11
      COMMON/CYL/R(30),RM(30),RMV(30),YSR(30),YSVR(30),IPLAX              COMMON    2
      COMMON/GRID/X(40),Y(30),Z(30),XS(40),YS(30),ZS(30),XSU(40),         COMMON    3
     1  YSV(30),ZSW(30),XDIF(40),YDIF(30),ZDIF(30),FXP(40),FXM(40),       COMMON    4
     2  FYP(30),FYM(30),FZP(30),FZM(30),DT,TIME                           COMMON    5
      COMMON                                                              NOX       2
     1/CINDEX/IDCO,IOFU,IDO2,IDN2,IDH2O,IDCO2,IDH1,IDH2,IDN1,IDNO,IDNO2   NOX       3
     1,IDO,IDOH,IHCPS,ILC,ILH,IMAT,ITER,JJJ,N1,N2,N3,NA,NGLOB,NGLOBP,     NOX       4
     2 NLM,NO,NSP,NS1,NS2,IDCH                                            4STEP     3
     3/CCHEMI/CPSUP,HSUN,FQ,PPLN,RGAS,RGASIN,SMINV,TKINV,TLN,LNRG         NOX       6
     4/CPARAM/ASUB(30,3),EMV,ER,HSUBO,NDEBUG,NS,PA,QQ,Q1,Q2,Q3,Q4,RHOPP,  NOX       7
     4 SM,SMW(30),SMO,S1(30),S2(30),TK,LADIAB,LDEBUG,LFQUIL,LREACT,       NOX       8
     4 LENER,EDRIJ,LCONVG                                                 NOX       9
      DOUBLE PRECISION CPSUN,EMV,ER,FQ,HSUBO,HSUM,PA,PPLN,QQ,Q1,Q2,Q3,    NOX      10
     1 Q4,RGAS,RGASIN,RHOPP,SM,SMINV,SMW,S1,S2,TK,TKINV,TLN,SMO           NOX      11
     2,FUT,FST                                                            4STEP     4
      COMMON/STEP4/PEXP1,PEXP2,PEXP3,PEXP4,ER1,ER2,ER3,ER4,CERU1,CERU2,   4STEP     5
     1 CERU3,CERU4,AEXP1,AEXP2,AEXP3,AEXP4,BEXP1,BEXP2,BEXP3,BEXP4,       4STEP     6
     2 CEXP1,CEXP2,CEXP3,CEXP4,FUT,FST                                    4STEP     7
      LOGICAL LADIAB,LCONVG,LDEBUG,LEQUIL,LNRG,LREACT,LENER                NOX      12
      COMMON/INT/L,M,N,LCV,MCV,NCV,LP1,MP1,NP1,NI,NJ,NK,NINJ,NINJNK,NV,    COMMON    6
     1 NNV,NGOTO,K,ISTR,JSTR,KSTR,NVM(35),KM(30),JM(30),ISTEP,            4STEP     8
     2 ISOLVE(32),IPRINT(33),TITLE(10,33),IXY,ISWP,JSWP,RELAX(35),NP,     4STEP     9
     3  NRHO,NGAM,IWLI(30,5),IWLO(30,5),JWLO(40,5),JWLI(40,5),IWFI,       COMMON    9
     4  IWFO,MM1,JWII,JWIO,JWOI,JWOO,IOW,JKIN(30,30),IKIN(40,30)          COMMON   10
      COMMON/INDEX/IPAR,LPREF,ISTUN,INCOMP,ITRAD,NVRX,NVRY,NVRZ,JPLANE    COMMON   11
     1,PLANM1,LVK,LVD,LVFUOX,LVFU,LVCO,LVH,LVRX,LVRY,LVRZ,NVF(32),        4STEP    10
     2  IJUMP,IREF,TITLE2(20),IMAX,JMAX,KMAX,NVCO,FUMCO,NVH2O,NVCO2,      COMMON   13
     3 NVN2,NVCH,NVH2                                                     4STEP    11
      COMMON/CNOX/LVH1,LVH2,LVN1,LVNO,LVNO2,LVO,LVOH,LVH2O,LVN2,LVO2,     NOX      16
     1 LVCO2,LVFU1,LVCO1,NNOX,INOX,ITNOX,SNOX,TNOX                        NOX      17
      COMMON/THERM/NVH,NVFU,NVOX,NVFUOX,NVTE,MODEN,IDK,FSTOIC,HFU,CP,     COMMON   15
     1  GASCON,RHOCON,UNICON,PRESS,NVFAV,TCYLW,TINLW,TLIP,ACOEF(4),       COMMON   16
     2  T4,OFAC,WFU,WCO2,WCO,WOX,WH2O,WN2,HYY,CXX,RATIO1,RATIO2,          COMMON   17
     3  RATIO3,RATIO4,HCO,TAN,ITWALL                                      COMMON   18
      COMMON/CTDMA/KEND,ICTDMA(32)                                        4STEP    12
      COMMON/MIS/AMU,DEN,SMAX,SSUM,LASTEP,HTCENT,CFR,EMISW,EMISIN,        COMGEN    2
     1  EMISR,TOUT,RTCO,EMI,RADIN,RADSUR,FMA,FK,SQFK,                     COMGEN    3
     2  FKFU,FDFU,TFUEL,WENZ,FLO(40),TEMTM(40),H(40),FUEL(40),FUOX(40) ,   COMGEN    4
     2 UIN(40),TIN(40),FUELS(40),SFXIT,IGAM1(29),IGAM2(29)                4STEP    13
      COMMON/TURB/NVK,NVD,C1,C2,CD,AK,DUIDXJ(3,3),AKFAC,ALFAC,            COMGEN    6
     1 MODEL,PR(32),PRFF(32),PJAY(32),E                                   4STEP    14
      COMMON/RAD/NVE,SIGMA,ARSOR,SCATR                                    COMGEN    8
      COMMON/REACT/ARCON1,PREXP1,CR1,ARCON2,PREXP2,CR2,MODER              COMGEN    9
      COMMON/DROPL/EVAP(192),NTP4,NENZ,X0(3),Y0(3),Z0(3),ALFA(3),         COMGEN   10
     1  BETA(3),DELTA(3),THETA1(3),THETA2(3),NSL(3),WFF(3),SMD(3),        COMGEN   11
     2  WFUEL(3),RFUEL(3),FVSU(64),HEVAP                                  COMGEN   12
      COMMON/INJEC/FLOWIN,IUINJ(20),JUINJ(20),UINJ(20),WUINJ(20),         COMGEN   13
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     1  AUINJ(20),TUINJ(20),IVINJ(20),JVINJ(20),KVINJ(20),VINJ(20),       COMGEN     14
     2  FVINJ(20),DVINJ(20),AVINJ(20),TVINJ(20),NUINJ,NVINJ,JSW1,JSW2,    COMGEN     15
     3  USW,VSW,AFSW,FSW,TSW,WSW,SWNO,RHOSW                               COMGEN     16
      COMMON/CSOOT/NVN,NVS1,NVS2,ISOOT,SSOOT,NSOOT,AO,ARCONN,AAA,BBB,FMG  SOOT       8
     1,GO,MPART,DPART(2),FRACP(2),RHOP,ARCONS,PREXPS,ALPHA,AAS,BBS,DHR   SOOT       9
     2,LVN,LVS1,LVS2,CINCP,TINCP,FUTOT                                   SOOT      10
      COMMON/CRAD/IRAD,SRAD                                              SOOT      11
      COMMON/CFOUR/PREXP3,ARCON3,CR3,PREXP4,ARCON4,CR4,AA1,BB1,CC1,      4STEP     15
     1 AA2,BB2,CC2,AA3,BB3,CC3,AA4,BB4,CC4,RATIO5,RATIO6,RATIO7,         4STEP     16
     2 RATIO8,RATIO9,RATO10,RATO11,RATO12,MCH,MH2,MC2H4,LVCH,LVCH1,LVH21 4STEP     17
      DIMENSION CLEND(2),CLENV(2),CENER(2),CMASS(2),CTEMP(2),CPRESS(2)    MA         7
      DIMENSION CANG(2)                                                  MA         8
      DATA CLEND/1.0,.0254/,CLENV/1.0,.3048/,CENER/1.0,1055./            MA         9
      DATA CMASS/1.0,.4536/,CTEMP/1.0,.55555/,CPRESS/1.0,101325./        MA        10
      DATA CANG/1.0,.01745/                                              MA        11
CHAPTER 1 ----------PARAMETERS AND CONTROL INDICES---------              MA        12
      NTP1=8                                                             MA        13
      NTP2=9                                                             MA        14
      NTP4=11                                                            MA        15
      READ (5,30) TITLE                                                  MA        16
      READ (5,31) TITLE2                                                 MA        17
   31 FORMAT (20A4)                                                      MA        18
   30 FORMAT (10A4)                                                      MA        19
      READ (5,100) LP1,MP1,NP1,IPLAX,MODEL,MODER,IPAR,ITRAD              MA        20
      READ (5,100) IU,MODEN,INTAPE,IDW,IRES                              MA        21
  100 FORMAT (8(I2,8X))                                                  MA        22
      READ (5,100) ISOLVE                                                MA        23
      READ (5,100) ICTDMA                                                MA        24
      READ (5,100) IPRINT                                                MA        25
      READ (5,101) RELAX                                                 MA        26
      READ (5,101) PR                                                    MA        27
      READ (5,101) PREF                                                  MA        28
  101 FORMAT (8E10.4)                                                    MA        29
      PLAXM1=FLOAT(IPLAX-1)                                              MA        30
CHAPTER 2 ----------GRID AND GEOMETRY----------                          MA        31
C+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+ MA        32
      CALL STRIDO                                                        MA        33
C+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+ MA        34
      READ (5,101) (X(I),I=1,LP1)                                        MA        35
      READ (5,101) (Y(J),J=1,MP1)                                        MA        36
      READ (5,101) (Z(K),K=1,NP1)                                        MA        37
      DO 200 I=1,LP1                                                     MA        38
  200 X(I)=X(I)*CLEND(IU)                                                MA        39
      DO 205 J=1,MP1                                                     MA        40
  205 Y(J)=Y(J)*CLEND(IU)                                                MA        41
      DO 220 K=1,NP1                                                     MA        42
      GO TO (210,215), IPLAX                                             MA        43
  210 Z(K)=Z(K)*CLEND(IU)                                                MA        44
      GO TO 220                                                          MA        45
  215 Z(K)=Z(K)*CANG(IU)                                                 MA        46
  220 CONTINUE                                                           MA        47
      RT=Y(1)                                                            MA        48
      Y(1)=0.0                                                           MA        49
C  ------  INCLINED WALL DATA                                           MA        50
      DO 22 J=1,MP1                                                      MA        51
      IWLI(J,4)=2                                                        MA        52
   22 IWLO(J,4)=L                                                        MA        53
      DO 26 J=1,LP1                                                      MA        54
      JWLI(J,4)=1                                                        MA        55
   26 JWLO(J,4)=MP1                                                      MA        56
      IWFO=L                                                             MA        57
      JWII=1                                                             MA        58
      JWOI=1                                                             MA        59
      JWOO=MP1                                                           MA        60
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```
      READ(5,100)IWEI,JWIO,IWEO,JWOO                                    NASAX      3
      IF (IWEI.EQ.2) GO TO 82                                            MA        62
      READ (5,100) (IWLI(J,4),J=JWIO,MP1)                                MA        63
      READ (5,100) (JWLO(I,4),I=1,IWEI)                                  MA        64
   82 CONTINUE                                                           MA        65
      IF(IWEO.EQ.L)GO TO 83                                              NASAX      4
      READ(5,100)(IWLO(J,4),J=JWOO,MP1)                                  NASAX      5
      READ(5,100)(JWLO(I,4),I=IWEO,LP1)                                  NASAX      6
   83 CONTINUE                                                           NASAX      7
      GO TO (23,24),IPAR                                                 MA        66
24    IREF=L                                                             MA        67
      JREF=M                                                             MA        68
      KREF=N                                                             MA        69
      LPREF=KM(KREF)+JM(JREF)+IREF                                       MA        70
23    CONTINUE                                                           MA        71
      DO 25 J=1,MP1                                                      MA        72
      GO TO (260,265), IPLAX                                             MA        73
  260 R(J)=1.0                                                           MA        74
      GO TO 25                                                           MA        75
  265 R(J)=RI+Y(J)                                                       MA        76
   25 CONTINUE                                                           MA        77
C+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+ MA        78
      CALL STRID1                                                        MA        79
C+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+ MA        80
CHAPTER 3 ----------------------------DEPENDENT VARIABLES-------------------- MA        81
      READ (5,101) PRESS,DEN,ABSOR,SCATR,AKFAC,ALFAC                     MA        82
      READ (5,101) CXX,HYY,HFU,FUNCO                                     MA        83
      READ (5,101) PREXP1,ARCON1,CR1,PREXP2,ARCON2,CR2                   MA        84
      READ(5,101)PREXP3,ARCON3,CR3,PREXP4,ARCON4,CR4                     4STEP     19
      READ(5,101)AA1,BB1,CC1,AA2,BB2,CC2                                 4STEP     20
      READ(5,101)AA3,BB3,CC3,AA4,BB4,CC4                                 4STEP     21
      READ (5,101) C1,C2,CD,AMU,ERROR,TCYLW,TINLW,TLIP                   MA        85
      READ (5,103) LASTFP,IJUMP,JSW1,JSW2,NUINJ,NVINJ                    MA        86
  103 FORMAT (2(I3,7X),6(I2,8X))                                         MA        87
      READ (5,101) USW,VSW,SWNO,AFSW,FSW,TSW                             MA        88
C-----FUEL INJECTION DATA.                                               COMMENT    1
      READ (5,102) NFN7,ISPRAY,TFUEL                                     MA        89
  102 FORMAT (2(I2,8X),6E10.4)                                           MA        90
      IF (NFN7.LE.C) GO TO 110                                           MA        91
      DO 115 I=1,NFN7                                                    MA        92
      READ (5,101) XO(I),YO(I),ZO(I),ALFA(I),BETA(I),DELTA(I),THETA1(I),  MA        93
     1  THETA2(I),RNSL,WFF(I),SMD(I),VFUEL(I),RFUEL(I)                   MA        94
  115 NSL(I)=IFIX(RNSL)                                                  MA        95
      DO 120 II=1,NFN7                                                   MA        96
      XO(II)=XO(II)*CLEND(IU)                                            MA        97
      YO(II)=YO(II)*CLEND(IU)                                            MA        98
      GO TO (125,130), IPLAX                                             MA        99
  125 ZO(II)=ZO(II)*CLEND(IU)                                            MA       100
      GO TO 135                                                          MA       101
  130 ZO(II)=ZO(II)*CANG(IU)                                             MA       102
  135 ALFA(II)=ALFA(II)*CANG(IU)                                         MA       103
      BETA(II)=BETA(II)*CANG(IU)                                         MA       104
      DELTA(II)=DELTA(II)*CANG(IU)                                       MA       105
      THETA1(II)=THETA1(II)*CANG(IU)                                     MA       106
      THETA2(II)=THETA2(II)*CANG(IU)                                     MA       107
      WFF(II)=WFF(II)*CMASS(IU)                                          MA       108
      RFUEL(II)=RFUEL(II)*CLEND(IU)                                      MA       109
  120 VFUEL(II)=VFUEL(II)*CLENV(IU)                                      MA       110
  110 CONTINUE                                                           MA       111
      TFUEL=TFUEL*CTEMP(IU)                                              MA       112
      AMU=AMU*CMASS(IU)/CLENV(IU)                                        MA       113
      PRESS=PRESS*CPRESS(IU)                                             MA       114
      DEN=DEN*CMASS(IU)/CLEND(IU)/CLEND(IU)/CLEND(IU)                    MA       115
      TCYLW=TCYLW*CTEMP(IU)                                              MA       116
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      TI4LW=TINLW*CTEMP(IU)                                              MA        117
      TLIP=TLIP*CTEMP(IU)                                                MA        118
      USW=USW*CLENV(IU)                                                  MA        119
      VSW=VSW*CLENV(IU)                                                  MA        120
      AFSW=AFSW*CMASS(IU)                                                MA        121
      FSW=FSW*CMASS(IU)                                                  MA        122
      TSW=TSW*CTEMP(IU)                                                  MA        123
C-----FILM COOLING DATA.                                                 COMMENT     2
      IF (NUINJ.LE.0) GO TO 85                                           MA        124
      READ (5,100) (IUINJ(I),I=1,NUINJ)                                  MA        125
      READ (5,100) (JUINJ(I),I=1,NUINJ)                                  MA        126
      READ (5,101) (UINJ(I),I=1,NUINJ)                                   MA        127
      READ (5,101) (WUINJ(I),I=1,NUINJ)                                  MA        128
      READ (5,101) (AUINJ(I),I=1,NUINJ)                                  MA        129
      READ (5,101) (TUINJ(I),I=1,NUINJ)                                  MA        130
      DO 295 II=1,NUINJ                                                  MA        131
      UINJ(II)=UINJ(II)*CLENV(IU)                                        MA        132
      WUINJ(II)=WUINJ(II)*CLENV(IU)                                      MA        133
      AUINJ(II)=AUINJ(II)*CMASS(IU)                                      MA        134
  295 TUINJ(II)=TUINJ(II)*CTEMP(IU)                                      MA        135
C-----DILUTION JET DATA.                                                 COMMENT     3
   85 IF (NVINJ.LE.0) GO TO 88                                           MA        136
      READ (5,100) (IVINJ(I),I=1,NVINJ)                                  MA        137
      READ (5,100) (JVINJ(I),I=1,NVINJ)                                  MA        138
      READ (5,100) (KVINJ(I),I=1,NVINJ)                                  MA        139
      READ (5,101) (VINJ(I),I=1,NVINJ)                                   MA        140
      READ (5,101) (EVINJ(I),I=1,NVINJ)                                  MA        141
      READ (5,101) (DVINJ(I),I=1,NVINJ)                                  MA        142
      READ (5,101) (AVINJ(I),I=1,NVINJ)                                  MA        143
      READ (5,101) (TVINJ(I),I=1,NVINJ)                                  MA        144
      DO 240 II=1,NVINJ                                                  MA        145
      VINJ(II)=VINJ(II)*CLENV(IU)                                        MA        146
      EVINJ(II)=EVINJ(II)*CLENV(IU)*CLENV(IU)                            MA        147
      DVINJ(II)=DVINJ(II)*CLENV(IU)                                      MA        148
      AVINJ(II)=AVINJ(II)*CMASS(IU)                                      MA        149
  240 TVINJ(II)=TVINJ(II)*CTEMP(IU)                                      MA        150
   88 READ(5,100)NSOOT,ISOOT,MPART                                       SOOT       13
C-----SOOT DATA.                                                         COMMENT     4
      IF(NSOOT.EQ.0)GO TO 910                                            SOOT       14
      READ(5,101)SSOOT,AO,ARCONN,AAA,BBB,FMG,GO,RHOP                     SOOT       15
      READ(5,101)PREXPS,ARCONS,ALPHA,AAS,BBS,DHR,CINCP,TINCP             SOOT       16
      READ(5,101)(DPART(I),I=1,MPART)                                    SOOT       17
      READ(5,101)(FRACP(I),I=1,MPART)                                    SOOT       18
      RHOP=RHOP*CMASS(IU)/(CLEND(IU)**3)                                 SOOT       19
      DHR=DHR*CENER(IU)/CMASS(IU)                                        SOOT       20
  910 CONTINUE                                                           SOOT       21
C-----RADIATION DATA.                                                    COMMENT     5
      IF(ITRAD.NE.1)READ(5,105)IRAD,SRAD                                 RAD         5
  105 FORMAT(I2,8X,E10.4)                                                RAD         6
C-----NOX DATA.                                                          COMMENT     6
      READ(5,104)NNOX,INOX,ITNOX,SNOX,TNOX                               NOX        22
  104 FORMAT(3(I2,8X),2E10.4)                                            NOX        23
      TNOX=TNOX*CTEMP(IU)                                                NOX        24
      CALL CREKO                                                         NOX        25
      WFU=12.*CXX+HYY                                                    MA        152
      ISTEP=IRES                                                         MA        153
      DFAC=1.0                                                           MA        154
      SUM1=.01                                                           MA        155
      SUM2=.05                                                           MA        156
CHAPTER 4 ----------MATERIAL CONSTANTS----------                         MA        157
      PREF(LVD)=AK*AK/(C2-C1)/SQRT(CD)                                   MA        158
      DO 93 NV=1,NNV                                                     MA        159
      PRRAT=PP(NV)/PREF(NV)                                              MA        160
   93 PJAY(NV)=E*(PRRAT-1.)/PRRAT**.25                                   MA        161
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      RHOCON=PRESS/UNICON                                                    MA        162
      GASCON=UNICON*(0.232/WOX+0.768/WN2)                                    NASAX       8
CHAPTER 5 ----------INITIAL VALUES----------                                 MA        164
      CALL START                                                             MA        165
      IF(INTAPE.NE.0)CALL OUTPUT(INTAPE)                                     NASAX       9
      JTRAD=ITRAD                                                            SOOT       22
      ITRAD=1                                                                SOOT       23
      JNOX=1                                                                 NOX        26
      SSUM=1.0E30                                                            SOOT       24
C---------- MAIN LOOP STARTS ----------                                      MA        167
60    CONTINUE                                                               MA        168
      IF(NSOOT.EQ.0)GO TO 64                                                 SOOT       25
C-----START SOOT CALCULATION.                                                COMMENT     7
      IF(ISTEP.LT.ISOOT.AND.SSUM.GT.SSOOT)GO TO 64                           SOOT       26
      DO 66 II=1,MPART                                                       SOOT       27
      ISOLVE(LVS1+II-1)=1                                                    SOOT       28
   66 IPRINT(29+II)=1                                                        SOOT       29
      ISOLVE(LVN)=1                                                          SOOT       30
      GO TO 63                                                               SOOT       31
   64 DO 67 II=1,MPART                                                       SOOT       32
      ISOLVE(LVS1+II-1)=0                                                    SOOT       33
   67 IPRINT(29+II)=0                                                        SOOT       34
      ISOLVE(LVN)=0                                                          SOOT       35
      IPRINT(23)=0                                                           SOOT       36
   63 IF(JTRAD.EQ.1)GO TO 65                                                 RAD         7
C-----START RADIATION CALCULATION.                                           COMMENT     8
      IF(ISTEP.GE.IRAD.OR.SSUM.LE.SRAD)ITRAD=JTRAD                           SOOT       38
      IF(ITRAD.EQ.1)GO TO 65                                                 RAD         8
      ISOLVE(LVRX)=1                                                         RAD         9
      ISOLVE(LVRY)=1                                                         RAD        10
      ISOLVE(LVRZ)=1                                                         RAD        11
      IPRINT(11)=1                                                           RAD        12
      IPRINT(12)=1                                                           RAD        13
      IPRINT(13)=1                                                           RAD        14
      IPRINT(14)=1                                                           RAD        15
      GO TO 69                                                               RAD        16
   65 CONTINUE                                                               SOOT       39
      ISOLVE(LVRX)=0                                                         RAD        17
      ISOLVE(LVRY)=0                                                         RAD        18
      ISOLVE(LVRZ)=0                                                         RAD        19
      IPRINT(11)=0                                                           RAD        20
      IPRINT(12)=0                                                           RAD        21
      IPRINT(13)=0                                                           RAD        22
      IPRINT(14)=0                                                           RAD        23
   69 CONTINUE                                                               RAD        24
      IF(JNOX.EQ.0)GO TO 70                                                  NOX        27
C-----START NOX CALCULATION.                                                 COMMENT     9
      IF(NNOX.EQ.0)GO TO 68                                                  NOX        28
      IF(ISTEP.LT.INOX.AND.SSUM.GT.SNOX)GO TO 68                             NOX        29
      ISOLVE(LVFU)=0                                                         NOX        30
      ISOLVE(LVCO)=0                                                         NOX        31
      ISOLVE(LVCH)=0                                                         4STEP      22
      ISOLVE(LVH2)=0                                                         4STEP      23
      ISOLVE(LVH1)=1                                                         NOX        32
      JNOX=0                                                                 NOX        33
      INOX=ISTEP                                                             NOX        34
      GO TO 70                                                               NOX        35
   68 ISOLVE(LVH1)=0                                                         NOX        36
   70 CONTINUE                                                               NOX        37
C+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-  MA        169
      IF (ISTEP.EQ.100) ISOLVE(LVK)=9                                        MA        170
      IF (ISTEP.EQ.100) ISOLVE(LVD)=9                                        MA        171
      CALL DENS                                                              MA        172
      ISP=ISPRAY                                                             MA        173
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      IF (ISTEP-IRES.LE.5) ISP=1                                          MA        174
      IF (MOD(ISTEP-IRES,ISP).EQ.0) CALL SPRAY                            MA        175
      CALL VISCO                                                          MA        176
C+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+- MA        177
CHAPTER 6  ----------------SINGLE LINE PRINTOUT----------------------     MA        178
      IF (ISTEP.EQ.IRES) GO TO 16                                         MA        179
      WRITE (6,10) ISTEP,SMAX,SSUM,SEXIT,P(2,M,2),P(L,M,2),               MA        180
     1  U(IMAX,JMAX,KMAX),V(IMAX,JMAX,KMAX),W(IMAX,JMAX,KMAX),            MA        181
     2  TEMP(IMAX,JMAX,KMAX),RHO(IMAX,JMAX,KMAX),IMAX,JMAX,KMAX           MA        182
   10 FORMAT (1X,I4,10(1PE11.3),1X,3I3)                                   MA        183
   16 CONTINUE                                                            MA        184
C+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+- MA        185
      CALL STRID2                                                         MA        186
C+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+- MA        187
CHAPTER 7  ----------------------OUTPUT-------------------------------    MA        188
      IF (ERROR.GT.SSUM) ISTEP=LASTEP                                     MA        189
      DFAC=AMAX1(0.,(SUM2-SSUM)/(SUM2-SUM1))                              MA        190
      DFAC=AMIN1(1.0,DFAC)                                                MA        191
      CALL OUTPUT (NTP1)                                                  MA        192
CHAPTER 8  ------------------TERMINATION ------------------------         MA        193
      IF (ISTEP-LASTEP) 60,80,80                                          MA        194
   80 WRITE (6,10) ISTEP,SMAX,SSUM                                        MA        195
C +-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+- MA        196
      STOP                                                                MA        197
      END                                                                 MA        198
      BLOCK DATA                                                          MA        199
      COMMON/CYL/R(30),RM(30),RMV(30),YSR(30),YSVR(30),IPLAX              COMMON      2
      COMMON/GRID/X(40),Y(30),Z(30),XS(40),YS(30),ZS(30),XSU(40),         COMMON      3
     1  YSV(30),ZSW(30),XDIF(40),YDIF(30),ZDIF(30),FXP(40),FXM(40),       COMMON      4
     2  FYP(30),FYM(30),FZP(30),FZM(30),DT,TIME                           COMMON      5
      COMMON                                                              NOX         2
     1/CINDEX/IDCO,IOFU,IDO2,IDN2,IOH2O,IDCO2,IOH1,IOH2,ION1,IONO,IONO2   NOX         3
     1,IDO,IOOH,IHCPS,ILC,ILH,IMAT,ITER,JJJ,N1,N2,N3,NA,NGLOB,NGLORP,     NOX         4
     2 NLM,NO,NSM,NS1,NS2,IOCH                                            4STEP       3
     3/CCHEMI/CPSUM,HSUM,FQ,PPLN,RGAS,RGASIN,SMINV,TKINV,TLN,LNRG         NOX         6
     4/CPARAM/ASUB(30,3),EMV,ER,HSUBO,NDEBUG,NS,PA,QQ,Q1,Q2,Q3,Q4,RHOPP,  NOX         7
     4 SM,SMW(30),SMO,S1(30),S2(30),TK,LADIAB,LDEBUG,LEQUIL,LREACT,       NOX         8
     4 LENER,RONIJ,LCONVG                                                 NOX         9
      DOUBLE PRECISION CPSUM,EMV,ER,FQ,HSUBO,HSUM,PA,PPLN,QQ,Q1,Q2,Q3,    NOX        10
     1 Q4,RGAS,RGASIN,RHOPP,SM,SMINV,SMW,S1,S2,TK,TKINV,TLN,SMO           NOX        11
     2,FUT,FST                                                            4STEP       4
      COMMON/STEP4/PEXP1,PEXP2,PEXP3,PEXP4,ER1,ER2,ER3,ER4,CEBU1,CEBU2,   4STEP       5
     1 CEBU3,CEBU4,AEXP1,AEXP2,AEXP3,AEXP4,BEXP1,BEXP2,BEXP3,BEXP4,       4STEP       6
     2 CEXP1,CEXP2,CEXP3,CEXP4,FUT,FST                                    4STEP       7
      LOGICAL LADIAB,LCONVG,LDEBUG,LEQUIL,LNRG,LREACT,LENER               NOX        12
      COMMON/INT/L,M,N,LCV,MCV,NCV,LP1,MP1,NP1,NI,NJ,NK,NIMJ,NIMJNK,NV,   COMMON      6
     1 NNV,NGOTO,K,ISTR,JSTR,KSTR,NVM(35),KM(30),JM(30),ISTEP,            4STEP       8
     2 ISOLVE(32),IPRINT(33),TITLE(10,3),IXY,ISWP,JSWP,RELAX(35),NP,      4STEP       9
     3  NRHO,NGAM,IWLI(30,5),IWLO(30,5),JWLO(40,5),JWLI(40,5),IWEI,       COMMON      9
     4  IWEO,PP1,JWII,JWIO,JWOI,JWOO,IDM,JKIN(30,30),IKIN(40,30)          COMMON     10
      COMMON/INDEX/IPAR,LPREF,ISTUN,INCOMP,ITRAD,NVRX,NVRY,NVRZ,JPLANE    COMMON     11
     1,PLAXM1,LVM,LVD,LVFUOX,LVFU,LVCO,LVH,LVRX,LVRY,LVRZ,NVF(32),        4STEP      10
     2  IJUMP,IRES,TITLE2(20),IMAX,JMAX,KMAX,NVCO,FUNCO,NVH2O,NVCO2,      COMMON     13
     3 NVN2,NVCH,NVH2                                                     4STEP      11
      COMMON/CNOX/LVH1,LVH2,LVN1,LVNO,LVNO2,LVO,LVOH,LVH2O,LVN2,LVO2,     NOX        16
     1 LVCO2,LVFU1,LVCO1,NNOX,INOX,ITNOX,SNOX,TNOX                        NOX        17
      COMMON/THERM/NVH,NVFU,NVOX,NVFUOX,NVTE,MODEN,IDK,FSTOIC,HFU,CP,     COMMON     15
     1  GASCON,RHOCON,UNICON,PRESS,NVFAV,TCYLW,TINLW,TLIP,ACOEF(4),       COMMON     16
     2  T4,DFAC,WFU,WCO2,WCO,WOX,WH2O,WN2,HYY,CXX,RATIO1,RATIO2,          COMMON     17
     3  RATIO3,RATIO4,HCO,TAN,ITWALL                                      COMMON     18
      COMMON/CTOMA/KEND,ICTOMA(32)                                        4STEP      12
      COMMON/MIS/AMU,DEN,SMAX,SSUM,LASTEP,HTCEXT,CFR,EMISW,EMISIN,        COMGEN      2
     1  EMISP,TOUT,RTCO,EMI,RADIN,RADSUR,FMA,FR,SOEK,                     COMGEN      3
     2  FXFU,FOFU,TFUEL,WFN2,FLO(40),TEMTM(40),H(40),FUEL(40),FUOX(40) ,   COMGEN      4
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     2 UIN(40),TIN(40),FUELS(40),SEXIT,IGAM1(29),IGAM2(29)                4STEP    13
      COMMON/TURB/NVK,NVD,C1,C2,CD,AK,DUIDXJ(3,3),AKFAC,ALFAC,            COMGEN    6
     1 MODEL,PR(32),PREF(32),PJAY(32),E                                   4STEP    14
      COMMON/RAD/NVE,SIGMA,ABSOR,SCATR                                    COMGEN    8
      COMMON/REACT/ARCON1,PREXP1,CR1,ARCON2,PREXP2,CR2,MODER              COMGEN    9
      COMMON/DROPL/EVAP(192),NTP4,NFNZ,XO(3),YO(3),ZO(3),ALFA(3),         COMGEN   10
     1   BETA(3),DELTA(3),THETA1(3),THETA2(3),NSL(3),WFF(3),SND(3),       COMGEN   11
     2   VFUEL(3),RFUEL(3),EVSU(64),HEVAP                                 COMGEN   12
      COMMON/INJEC/FLOWIN,IUINJ(20),JUINJ(20),UINJ(20),WUINJ(20),         COMGEN   13
     1   AUINJ(20),TUINJ(20),IVINJ(20),JVINJ(20),KVINJ(20),VINJ(20),      COMGEN   14
     2   EVINJ(20),DVINJ(20),AVINJ(20),TVINJ(20),NUINJ,NVINJ,JSW1,JSW2,   COMGEN   15
     3   USW,VSW,AFSW,FSW,TSW,WSW,SWNO,RHOSW                              COMGEN   16
      COMMON/CSOOT/AVN,NVS1,NVS2,ISOOT,SSOOT,NSOOT,AD,ARCONN,AAA,BBB,FNG   SOOT     8
     1,GO,MPART,DPART(2),FRACP(2),RHOP,ARCONS,PREXPS,ALPHA,AAS,BBS,DHR     SOOT     9
     2,LVN,LVS1,LVS2,CINCP,TINCP,FUTOT                                     SOOT    10
      COMMON/CRAD/IRAD,SRAD                                               SOOT    11
      COMMON/CFOUR/PREXP3,ARCON3,CR3,PREXP4,ARCON4,CR4,AA1,BB1,CC1,       4STEP    15
     1 AA2,BB2,CC2,AA3,BB3,CC3,AA4,BB4,CC4,RATIO5,RATIO6,RATIO7,          4STEP    16
     2 RATIO8,RATIO9,RATO10,RATO11,RATO12,WCH,WH2,WC2H4,LVCH,LVCH1,LVH21  4STEP    17
      DATA NI,NJ,NK,NNV/10,10,5,29/                                       4STEP    24
      DATA AK,E/.43,9./                                                   MA      203
      DATA UNICON,SIGMA/8314.,5.669E-08/                                  MA      204
      DATA NVK,NVD,NVFUOX,NVFU,NVCH,NVCO,NVH2,NVTE,NVH,NVN,NVS1,NVS2      4STEP    25
     1/4,5,4,5,14,8,15,6,9,11,12,13/                                      4STEP    26
      DATA NVFAV,NVRX,NVRY,NVRZ/10,1,2,3/                                 MA      206
      DATA IDFU,IDC2,IDN2,IDCO,IDCH,IDH2,IDH2O,IDCO2,IDH1,IDN1,IDNO,      4STEP    27
     1 IDNO2,IDO,IDOH/1,2,3,4,5,6,7,8,9,10,11,12,13,14/                   4STEP    28
      DATA NVF/1,2,3,4,4,5,4,5,14,8,15,9,11,12,13,16,17,18,19,20,21,22,   4STEP    29
     1 23,24,25,26,27,28,29,1,2,3/                                        4STEP    30
      DATA LVK,LVD,LVFUOX,LVFU,LVCH,LVCO,LVH2,LVH,LVN,LVS1,LVS2/5,6,      4STEP    31
     1 7,8,9,10,11,12,13,14,15/                                           4STEP    32
      DATA LVFU1,LVC2,LVN2,LVCO1,LVCH1,LVH21,LVH2O,LVCO2,LVH1,LVN1,       4STEP    33
     1 LVNO,LVNO2,LVO,LVOH/16,17,18,19,20,21,22,23,24,25,26,27,28,29/     4STEP    34
      DATA LVRX,LVRY,LVRZ/30,31,32/                                       4STEP    35
      DATA NVH2O,NVCX,NVCO2,NVN2/1,2,3,4/                                 MA      210
      DATA NP,NRHO,NGAM/33,34,35/                                         4STEP    36
      DATA WCO2,WCO,WOX,WH2O,WN2,WH2,WC2H4/44.,28.,32.,18.,28.,2.,28./    4STEP    37
      DATA IGAM1,IGAM2/1,0,3*1,24*0,0,4*1,24*0/                           4STEP    38
      DATA ACOEF/-1306.01,8620.37,-6167.08,1336.65/                       MA      214
      END                                                                 MA      215
      SUBROUTINE INIT                                                     MASAX    10
      COMMON F(500,7),DU(10,10,5),DV(10,10,5),DW(10,10,5),                COMFA     2
     1 ANUC(10,10,5),SOOT1(10,10,5),SOOT2(10,10,5),FCH(10,10,5),          4STEP     1
     2 FH2(10,10,5),FS(500,14),                                           4STEP     2
     1 RHO(10,10,5),VISC(10,10,5),ABSR(10,10,5),SCTR(10,10,5),            RAD       1
     1 SU(10,10),SP(10,10),DRHODP(10,10,5),                               RAD       2
     1   AXP(10,10),AXM(10,10),AYP(10,10),AYM(10,10),AZP(10,10),          COMFA     4
     2   AZM(10,10),CZ(10,10),CY(10),CZU(10,10),CYU(10),                  COMFA     5
     3   CZP(10,10),CYP(10),DIVG(10,10),NTP1,NTP2                         COMFA     6
     1,AXMK(192),AXPK(192),AYMK(192),AYPK(192),AZMK(192),AZPK(192),       CTOMA     1
     2 SUK(192),SPK(192)                                                  CTOMA     2
      DIMENSION U(10,10,5),V(10,10,5),W(10,10,5),PP(10,10,5)              COMFA     7
      DIMENSION P(10,10,5),TEMP(10,10,5),GAM(10,10,5)                     COMFA     8
      EQUIVALENCE (F(1,1),U(1,1,1)),(F(1,2),V(1,1,1)),(F(1,3),W(1,1,1))   COMFA     9
      EQUIVALENCE (F(1,4),PP(1,1,1)),(F(1,5),P(1,1,1))                    COMFA    10
      EQUIVALENCE (F(1,6),TEMP(1,1,1)),(F(1,7),GAM(1,1,1))                COMFA    11
      COMMON/CYL/R(30),RM(30),RMV(30),YSR(30),YSVR(30),IPLAX              COMMON    2
      COMMON/GRID/X(40),Y(30),Z(30),XS(40),YS(30),ZS(30),XSU(40),         COMMON    3
     1   YSV(30),ZSW(30),XDIF(40),YDIF(30),ZDIF(30),FXP(40),FXM(40),      COMMON    4
     2   FYP(30),FYM(30),FZP(30),FZM(30),DT,TIME                          COMMON    5
      COMMON
     1/CINDEX/IDCO,IDFU,IDO2,IDN2,IDH2O,IDCO2,IDH1,IDH2,IDN1,IDNO,IDNO2   NOX       2
     1,IDO,IDOH,IHCPS,ILC,ILH,IRAT,ITER,JJJ,N1,N2,N3,NA,NGLOB,NGLOBP,     NOX       3
     2 NLM,NQ,NSM,NS1,NS2,IDCH                                            NOX       4
                                                                          4STEP     3
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     3/CCHEMI/CPSUM,HSUM,FQ,PPLN,RGAS,RGASIN,SMINV,TKINV,TLN,LNRG          NOX          6
     4/CPARAM/ASUB(30,3),EMV,ER,HSUBO,NDEBUG,NS,PA,QQ,Q1,Q2,Q3,Q4,RHOPP,  NOX          7
     4 SM,SMW(30),SPO,S1(30),S2(30),TK,LADIAB,LDEBUG,LEQUIL,LREACT,       NOX          8
     4 LENER,FDKID,LCONVG                                                 NOX          9
      DOUBLE PRECISION CPSUM,EMV,ER,FQ,HSUBO,HSUM,PA,PPLN,QQ,Q1,Q2,Q3,    NOX         10
     1 Q4,RGAS,RGASIN,RHOPP,SM,SMINV,SMW,S1,S2,TK,TKINV,TLN,SMO           NOX         11
     2,FUT,FST                                                            4STEP        4
      COMMON/STEP4/PEXP1,PEXP2,PEXP3,PEXP4,ER1,ER2,ER3,ER4,CEBU1,CEBU2,   4STEP        5
     1 CEBU3,CEBU4,AEXP1,AEXP2,AEXP3,AEXP4,BEXP1,BEXP2,BEXP3,BEXP4,       4STEP        6
     2 CEXP1,CEXP2,CEXP3,CEXP4,FUT,FST                                    4STEP        7
      LOGICAL LADIAB,LCONVG,LDEBUG,LEQUIL,LNRG,LREACT,LENER               NOX         12
      COMMON/INT/L,M,N,LCV,MCV,NCV,LP1,MP1,NP1,MI,NJ,NK,NINJ,NINJNK,NV,   COMMON       6
     1 NNV,NGOTO,K,ISTR,JSTR,KSTR,NVN(35),KM(30),JM(30),ISTEP,            4STEP        8
     2 ISOLVE(32),IPRINT(38),TITLE(10,3),IXY,ISWP,JSWP,RELAX(35),NP,      4STEP        9
     3  NRHO,NGAM,IWLI(30,5),IWLO(30,5),JWLO(40,5),JWLI(40,5),IWFI,       COMMON       9
     4  IWEO,MM1,JWII,JWIO,JWOI,JWOO,IOW,JKIN(30,30),IKIN(40,30)          COMMON      10
      COMMON/INDEX/IPAR,LCREF,ISTUN,INCOMP,ITRAD,NVRX,NVRY,NVRZ,JPLANE    COMMON      11
     1,PLAXM1,LVK,LVD,LVFUOX,LVFU,LVCO,LVH,LVRX,LVRY,LVRZ,NVF(32),        4STEP       10
     2  IJUMP,IRES,TITLE2(20),IMAX,JMAX,KMAX,NVCO,FUMCO,NVH2O,NVCO2,      COMMON      13
     3 NVN2,NVCH,NVH2                                                     4STEP       11
      COMMON/CNOX/LVH1,LVH2,LVN1,LVNO,LVNO2,LVO,LVOH,LVH2O,LVN2,LVO2,     NOX         16
     1 LVCO2,LVFU1,LVCO1,NNOX,INOX,ITNOX,SNOX,TNOX                        NOX         17
      COMMON/THERM/NVH,NVFU,NVOX,NVFUOX,NVTE,NODEN,IDK,FSTOIC,HFU,CP,     COMMON      15
     1  GASCON,RHOCON,UNICON,PRESS,NVFAV,TCYLW,TINLW,TLIP,ACOEF(4),       COMMON      16
     2  T4,DFAC,WFU,WCO2,WCO,WOX,WH2O,WN2,HYY,CXX,RATIO1,RATIO2,          COMMON      17
     3  RATIO3,RATIO4,HCO,TAN,ITWALL                                      COMMON      18
      COMMON/CTOMA/KEND,ICTOMA(32)                                        4STEP       12
      COMMON/MIS/AMU,DEN,SMAX,SSUM,LASTEP,HTCEXT,CFR,EMISW,EMISIN,        CONGEN       2
     1  EMISR,TOUT,RTCO,SNI,RADIN,RADSUR,FMA,FK,SOFK,                     CONGEN       3
     2  FKFU,FOFU,TFUEL,WFN2,FLO(40),TEMTM(40),H(40),FUEL(40),FUOX(40) ,   CONGEN       4
     2 UIN(40),TIN(40),FUELS(40),SEXIT,IGAM1(29),IGAM2(29)                4STEP       13
      COMMON/TURB/NVK,NVD,C1,C2,CO,AK,DUIDXJ(3,3),AKFAC,ALFAC,            CONGEN       6
     1 MODEL,PR(32),PREF(32),PJAY(32),E                                   4STEP       14
      COMMON/RAD/NVE,SIGMA,ABSOR,SCATR                                    CONGEN       8
      COMMON/REACT/ARCON1,PREXP1,CR1,ARCON2,PREXP2,CR2,MODER              CONGEN       9
      COMMON/DROPL/EVAP(192),NTP4,NFN7,XO(3),YO(3),ZO(3),ALFA(3),         CONGEN      10
     1  BETA(3),DELTA(3),THETA1(3),THETA2(3),NSL(3),WFF(3),SND(3),        CONGEN      11
     2  VFUEL(3),RFUEL(3),EVSU(64),HEVAP                                  CONGEN      12
      COMMON/INJEC/FLOWIN,IUINJ(20),JUINJ(20),UINJ(20),WUINJ(20),         CONGEN      13
     1  AUTNJ(20),TUINJ(20),IVINJ(20),JVINJ(20),KVINJ(20),VINJ(20),       CONGEN      14
     2  EVINJ(20),DVINJ(20),AVINJ(20),TVINJ(20),NUINJ,NVINJ,JSW1,JSW2,    CONGEN      15
     3  USW,VSW,AFSW,FSW,TSW,WSW,SWND,RHOSW                               CONGEN      16
      COMMON/CSOOT/MVN,NVS1,NVS2,ISOOT,SSOOT,NSOOT,AO,ARCONN,AAA,BBB,FMG  SOOT         8
     1,GO,MPART,DPART(2),FRACP(2),RHOP,ARCONS,PREXPS,ALPHA,AAS,BBS,OMR    SOOT         9
     2,LVN,LVS1,LVS2,CINCP,TINCP,FUTOT                                    SOOT        10
      COMMON/CRAD/IRAD,SRAD                                               SOOT        11
      COMMON/CFOUR/PREXP3,ARCON3,CR3,PREXP4,ARCON4,CR4,AA1,BB1,CC1,       4STEP       15
     1 AA2,BB2,CC2,AA3,BB3,CC3,AA4,BB4,CC4,RATIO5,RATIO6,RATIO7,          4STEP       16
     2 RATIO8,RATIO9,RATO10,RATO11,RATO12,WCH,WH2,WC2H4,LVCH,LVCH1,LVH21  4STEP       17
C  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  AL           7
      ENTRY START                                                         AL           8
C-----SUBROUTINE INIT(ENTRY START) IS USED FOR INITIALIZATION PURPOSES.    COMMENT     10
C  ------------   SOME PRELIMINARY VALUES   ---------------------         AL           9
      HCO=1.0112E+7                                                       AL          10
      RATIO1=WOX*(CXX+HYY/4.)/WFU                                         AL          11
      RATIO2=.232                                                         AL          12
      RATIO3=WOX*0.5/WCO                                                  AL          13
      RATIO4=WCO*CXX/WFU                                                  AL          14
      WCH=12.01*CXX+1.008*(HYY-2.0)                                       4STEP       39
      SMW(IDCH)=WCH                                                       4STEP       40
      RATIO5=(CXX+(HYY-2.0)*.25)*WOX/WCH                                  4STEP       41
      RATIO6=0.25*WCH                                                     4STEP       42
      RATIO7=(HYY-2.0)/WCH                                                4STEP       43
      RATIO8=WCH/WFU                                                      4STEP       44
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      RATIO9=HYY*WH2/(2.0*WFU)                                          4STEP    45
      RATIO10=(HYY-2.0)*WH2/(2.0*WCH)                                   4STEP    46
      RATIO11=CXX*WCO/WCH                                               4STEP    47
      RATIO12=WH2/WFU                                                   4STEP    48
      FSTOIC=RATIO2/(RATIO1+RATIO2)                                     AL       15
      WFU=WFU/1.987                                                     NOX      48
      CFR=.003                                                          AL       18
      EMISW=.0                                                          AL       19
      EMISIN=1.                                                         AL       20
      EMISR=1.                                                          AL       21
      UMASS=0.                                                          AL       22
      SMASS=1.E-30                                                      AL       23
      ASW=AFSW-FSW                                                      AL       24
      FUMSW=FSW/AFSW                                                    AL       25
      FUMXSW=FUMSW                                                      AL       26
      WSW=SWNO*USW                                                      AL       27
      UMASS=AFSW*USW                                                    AL       28
      SMASS=AFSW                                                        AL       29
      FK=AMAX1(10.,AKFAC*(UMASS/SMASS)**2)*FLOAT(MODEL-1)               AL       30
      SQFK=SQRT(FK)                                                     AL       31
      ASWRLR=0.                                                         AL       32
      DO 10 J=JSW1,JSW2                                                 AL       33
   10 ASWRLR=ASWRLR+YSP(J)*(Z(NP1)-Z(1))                                AL       34
      ALIN=.5*ALFAC*(Y(JSW2)+Y(JSW2+1)-Y(JSW1)+Y(JSW1-1))               AL       35
      RHOSW=AFSW/ASWRLR/USW                                             AL       36
      RTCO=SQRT(CO)                                                     AL       37
      DO 40 I=1,LP1                                                     AL       38
   40 FUELS(I)=0.                                                       AL       39
C-----FUEL INJECTION.                                                  COMMENT  11
      IF (NFNZ.LE.0) GO TO 48                                           AL       40
      DO 165 II=1,NFNZ                                                  AL       41
      DO 165 I=2,L                                                      AL       42
      IF (XO(II).GT.0.5*(X(I)+X(I+1))) GO TO 165                        AL       43
      FUELS(I)=FUELS(I)+WFF(II)                                         AL       44
  165 CONTINUE                                                          AL       45
   48 FUELS(LP1)=FUELS(L)                                               AL       46
      WFNZ=FUELS(LP1)                                                   AL       47
C-----BOUNDARY CONDITIONS.                                             COMMENT  12
      DO 80 K=1,NP1                                                     AL       48
      DO 82 J=1,MP1                                                     AL       49
   82 JKIN(J,K)=0                                                       AL       50
      DO 80 I=1,LP1                                                     AL       51
   80 IKIN(I,K)=0                                                       AL       52
      DO 86 K=1,NP1                                                     AL       53
      DO 86 J=JSW1,JSW2                                                 AL       54
   86 JKIN(J,K)=1                                                       AL       55
   84 CONTINUE                                                          AL       56
C-----DILUTION JETS.                                                   COMMENT  13
   88 IF (NVINJ.LE.0) GO TO 92                                          AL       57
      DO 94 II=1,NVINJ                                                  AL       58
      I=IVINJ(II)                                                       AL       59
      J=JVINJ(II)                                                       AL       60
      K=KVINJ(II)                                                       AL       61
      IF (J.EQ.JWLI(I,4)) GO TO 96                                      AL       62
      IKIN(I,K)=IKIN(I,K)+2                                             AL       63
      GO TO 94                                                          AL       64
   96 IKIN(I,K)=IKIN(I,K)+1                                             AL       65
   94 CONTINUE                                                          AL       66
C-----FILM COOLING SLOTS.                                              COMMENT  14
   92 IF (NUINJ.LE.0) GO TO 199                                         AL       67
      DO 198 II=1,NUINJ                                                 AL       68
      I=IUINJ(II)-1                                                     AL       69
      J=JUINJ(II)                                                       AL       70
      IF (J.EQ.JWLI(I,4)+1) GO TO 197                                   AL       71
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      DO 196 K=1,NP1                                                    AL        72
  196 IKIN(I,K)=IKIN(I,K)+2                                             AL        73
      GO TO 198                                                         AL        74
  197 DO 195 K=1,NP1                                                    AL        75
  195 IKIN(I,K)=IKIN(I,K)+1                                             AL        76
  198 CONTINUE                                                          AL        77
  199 CONTINUE                                                          AL        78
C  ------    COMPUTE TOTAL FLOW RATE  ------------------------         AL        79
   94 DO 499 I=1,LP1                                                    AL        80
      FLO(I)=0.                                                         AL        81
      FUEL(I)=0.                                                        AL        82
  499 TEMTM(I)=0.                                                       AL        83
      FLO(1)=AFSW                                                       AL        84
      FUEL(1)=FSW                                                       AL        85
      TEMTM(1)=AFSW*TSW                                                 AL        86
C -------- AXIAL INJECTION                                            AL        87
      IF (NUINJ.LE.0) GO TO 104                                         AL        88
      DO 106 II=1,NUINJ                                                 AL        89
      I=IUINJ(II)-1                                                     AL        90
      FLO(I)=FLO(I)+AUINJ(II)                                           AL        91
  106 TEMTM(I)=TEMTM(I)+TUINJ(II)*AUINJ(II)                             AL        92
C -------- RADIAL INJECTION                                           AL        93
  104 IF (NVINJ.LE.0) GO TO 108                                         AL        94
      DO 110 II=1,NVINJ                                                 AL        95
      I=IVINJ(II)                                                       AL        96
      FLO(I)=FLO(I)+AVINJ(II)                                           AL        97
  110 TEMTM(I)=TEMTM(I)+TVINJ(II)*AVINJ(II)                             AL        98
  108 CONTINUE                                                          AL        99
C -------- FLOW RATE AT EACH I-STATION                                AL       100
      DO 139 I=2,LP1                                                    AL       101
      FLO(I)=FLO(I-1)+FLO(I)                                            AL       102
      FUEL(I)=FUEL(I-1)+FUEL(I)                                         AL       103
  139 TEMTM(I)=TEMTM(I-1)+TEMTM(I)                                      AL       104
      FLOWIN=FLO(LP1)+WFNZ                                              AL       105
      DO 145 I=1,LP1                                                    AL       106
  145 FUMX(I)=FUEL(I)/FLO(I)                                            AL       107
      FUTOT=FUEL(LP1)+WFNZ                                              AL       108
      AMASS=FLO(LP1)-FUEL(LP1)                                          AL       109
      FUARAT=FUTOT/AMASS                                                AL       110
      DO 150 I=1,LP1                                                    AL       111
      FUELI=(FUEL(I)+FUELS(I))/(FLO(I)+FUELS(I))                        AL       112
      FUELF=AMAX1(FUELI-RATIO2*(1.-FUELI)/RATIO1,0.)                    AL       113
      PHI=FUELI/FSTOIC                                                  AL       114
      IHCPS=9                                                           NOX       49
      NS1=IDFU                                                          NOX       50
      NS2=IDN2                                                          NOX       51
      TK=TSW                                                            NOX       52
      TKINV=1.000/TK                                                    NOX       53
      S2(IDFU)=FUELI/SMW(IDFU)                                          NOX       54
      S2(IDO2)=(1.0-FUELI)*RATIO2/SMW(IDO2)                             NOX       55
      S2(IDN2)=(1.0-FUELI)*(1.0-RATIO2)/SMW(IDN2)                       NOX       56
      CALL HCPS                                                         NOX       57
      H1=HSUM*UNICON*TK                                                 NOX       58
      TIN(I)=TSW                                                        AL       117
      FUB=FUELI-FUELF                                                   AL       118
      FLPCO2=WCO2*(CXX*FUB/WFU-CXX*FUMCO/WCH-FUMCO/WCO)                 4STEP     49
      FLPOX=RATIO1*FUELF+RATIO3*FUMCO+RATIO2-(RATIO1+RATIO2)*FUELI      AL       120
     1+(RATIO5+RATIO6)*FUMCO                                           4STEP     50
      FLPOX=AMAX1(FLPOX,0.)                                             AL       121
      FLPH2O=0.5*WH2O*(HYY*FUB/WFU-(RATIO7+1.0)*FUMCO)                  4STEP     51
      FLPN2=1.0-FUELF-FLPCO2-3.0*FUMCO-FLPOX-FLPH2O                     4STEP     52
      IHCPS=4                                                           NOX       59
      NS1=IDFU                                                          NOX       60
      NS2=IDCO2                                                         NOX       61
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      S2(IDFU)=FUELF/SMW(IDFU)                                          NOX      62
      S2(IDO2)=FLPOX/SMW(IDO2)                                          NOX      63
      S2(IDN2)=FLPN2/SMW(IDN2)                                          NOX      64
      S2(IDCO)=FUMCO/SMW(IDCO)                                          NOX      65
      S2(IDCH)=FUMCO/SMW(IDCH)                                          4STEP    53
      S2(IDH2)=FUMCO/SMW(IDH2)                                          4STEP    54
      S2(IDH2O)=FLPH2O/SMW(IDH2O)                                       NOX      66
      S2(IDCO2)=FLPCO2/SMW(IDCO2)                                       NOX      67
C-----IGNITION SEQUENCE.                                                COMMENT  15
      DO 151 II=1,10                                                    AL      124
      T=TIN(I)                                                          AL      125
      TK=T                                                              NOX      68
      TKINV=1.0D0/TK                                                    NOX      69
      CALL HCPS                                                         NOX      70
      H2=HSUM*UNICON*TK                                                 NOX      71
      CPI=CPSUM*UNICON                                                  NOX      72
      TNEW=T+(H1-H2)/CPI                                                AL      130
      TMAX=ACOEF(1)+PHI*(ACOEF(2)+PHI*(ACOEF(3)+PHI*ACOEF(4)))          AL      131
      TMAX=AMAX1(TMAX,2000.)                                            AL      132
      TNEW=AMIN1(TNEW,TMAX)                                             AL      133
      IF (ABS(TIN(I)-TNEW).LT.10.) GO TO 150                            AL      134
  151 TIN(I)=TNEW                                                       AL      135
      WRITE (6,156)                                                     AL      136
  156 FORMAT (' **ERROR-100')                                           AL      137
  150 CONTINUE                                                          AL      138
      T4=TIN(LP1)                                                       AL      139
      IHCPS=1                                                           NOX      73
      NS1=IDO2                                                          NOX      74
      NS2=IDN2                                                          NOX      75
      TK=T4                                                             NOX      76
      TKINV=1.0D0/TK                                                    NOX      77
      S2(IDO2)=RATIO2/SMW(IDO2)                                         NOX      78
      S2(IDN2)=(1.0-RATIO2)/SMW(IDN2)                                   NOX      79
      CALL HCPS                                                         NOX      80
      CP=CPSUM*UNICON                                                   NOX      81
C-----AVERAGE U-VELOCITY AT EACH I-SECTION.                             COMMENT  16
      DO 231 I=3,LP1                                                    AL      141
      J1=JWL1(I,1)                                                      AL      142
      J2=JWL2(I,1)                                                      AL      143
      RHO4=PRESS/GASCON/TIN(I-1)                                        AL      144
      A4=.5*(Z(NP1)-Z(1))*(RM(J2)**2-RM(J1+1)**2)                       AL      145
      IF (IPLAN.EQ.2) GO TO 231                                         AL      146
      Y1=.5*(Y(J1)+Y(J1+1))                                             AL      147
      IF (J1.EQ.1) Y1=Y(J1)                                             AL      148
      Y2=.5*(Y(J2)+Y(J2-1))                                             AL      149
      IF (J2.EQ.NP1) Y2=Y(J2)                                           AL      150
      A4=(Z(NP1)-Z(1))*(Y2-Y1)                                          AL      151
  231 UIN(I)=FLO(I-1)/RHO4/A4                                           AL      152
      EMI=EMISW/(2.-EMISW)                                              AL      153
      RADIN=EMISIN*SIGMA*TSW**4                                         AL      154
      RADSUR=EMISR*SIGMA*T4**4                                          AL      155
C  --------   PRINTOUT INPUT DATA   ------------------------------      AL      156
      WRITE (6,1004) TITLE2                                             AL      157
 1004 FORMAT(1H1,24X,20A4/25X,80(1H-))                                  FEB2      1
      HCRAT=HYY/CXX                                                     AL      159
      WRITE (6,2010) HCRAT,WFU,HFU                                      AL      160
 2010 FORMAT (2X,'1.    PHYSICAL INPUT'/8X,14(1H-)/10X,'1.FUEL-'/       AL      161
     4  30X,'HYDROGEN-CARBON RATIO ----------',1PE12.4,/                AL      162
     2  30X,'MOLECULAR WEIGHT----------',1PE12.4,'  (KG/KGMOLE)'/       AL      163
     3  30X,'HEAT OF FORMATION----------',1PE12.4,'  (CAL/GMOLE)')      AL      164
      JJ=1                                                              AL      165
      WRITE (6,2014) JJ,FSW                                             AL      166
 2014 FORMAT (30X,'INLET-',I1,' MASS FLOW RATE----------',1PE12.4,      AL      167
     1  '  (KG/S)')                                                     AL      168
158
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      WRITE (6,2020) PRESS                                                  AL        169
 2020 FORMAT (10X,'2.AIR -'/                                                AL        170
     3  30X,'PRESSURE----------',1PE12.4,'  (NEW/SQ.M)')                    AL        171
      WRITE (6,2024) JJ,ASW,JJ,USW,JJ,SWNO                                  AL        172
 2024 FORMAT (30X,'INLET-',I1,' MASS FLOW RATE----------',1PE12.4,          AL        173
     1  '  (KG/S)'/30X,'INLET-',I1,' AXIAL VELOCITY----------',1PE12.4,     AL        174
     2  '  (M/S)'/30X,'INLET-',I1,' SWIRL NUMBER----------',                AL        175
     3  1PE12.4)                                                           AL        176
      HEIGHT=2.*(Y(MP1)-Y(1))                                               AL        177
      ALNGHT=X(LP1)-X(1)                                                    AL        178
      SECTOR=Z(NP1)-Z(1)                                                    AL        179
      WRITE (6,2025) HEIGHT,ALNGHT,SECTOR                                   AL        180
 2025 FORMAT (2X,'II.   GEOMETRICAL INPUT'/8X,18(1H-)/                      AL        181
     1  30X,'CHANNEL HEIGHT OF COMBUSTOR------',1PE12.4,'  (M)'/            AL        182
     2  30X,'LENGTH OF COMBUSTOR-----------',1PE12.4,'  (M)'/              AL        183
     2  30X,'ANGULAR SECTOR----------------',1PE12.4,'  (RAD-M)')          AL        184
      WRITE (6,2029) JJ,ASWRLR                                              AL        185
 2029 FORMAT (30X,'INLET-',I1,' FLOW AREA--------------',1PE12.4,           AL        186
     1  '  (SQ.M)')                                                        AL        187
      IF (NUINJ+NVINJ+NFNZ.GT.0) WRITE (6,2030)                             AL        188
 2030 FORMAT (2X,'III.  AIR INJECTIONS'/8X,14(1H-))                         AL        189
      IF (NUINJ.LE.0) GO TO 770                                             AL        190
      WRITE (6,2031)                                                        AL        191
 2031 FORMAT (10X,'1.FILM COOLING AIR-')                                    AL        192
      WRITE (6,2033)                                                        AL        193
 2033 FORMAT (25X,'SLOT NO',4X,'I',5X,'J',4X,'K',8X,'U-VELOCITY',           AL        194
     1  5X,'V-VELOCITY',5X,'W-VELOCITY',6X,'MASS FLOW',6X,'FUEL FLOW'/      AL        195
     2  49X,'(M/S)',10X,'(M/S)',10X,'(M/S)',10X,'(KG/S)',9X,'(KG/S)')      AL        196
      DO 772 II=1,NUINJ                                                     AL        197
      I=IUINJ(II)                                                           AL        198
      J=JUINJ(II)                                                           AL        199
  772 WRITE (6,2090) II,I,J,KUDEF,UINJ(II),UDEF,WUINJ(II),AUINJ(II)         AL        200
  770 IF (NVINJ.LE.0) GO TO 774                                             AL        201
      WRITE (6,2034)                                                        AL        202
 2034 FORMAT (/10X,'2.DILUTION AND SECONDARY AIR-')                         AL        203
      WRITE (6,2033)                                                        AL        204
      DO 776 II=1,NVINJ                                                     AL        205
      I=IVINJ(II)                                                           AL        206
      K=KVINJ(II)                                                           AL        207
      J=JVINJ(II)                                                           AL        208
  776 WRITE (6,2090) II,I,J,K,UDEF,VINJ(II),UDEF,AVINJ(II)                  AL        209
  774 CONTINUE                                                              AL        210
 2090 FORMAT (27X,I3,4X,I3,3X,I3,2X,I3,8X,1PE10.3,4(5X,1PE10.3))            AL        211
  810 IF (NFNZ.LE.0) GO TO 813                                              AL        212
      WRITE (6,816)                                                         AL        213
  816 FORMAT (/10X,'3.FUEL NOZZLES-'/12X,'XO',8X,'YO',8X,'ZO',6X,'ALFA',    AL        214
     1  6X,'BETA',5X,'DELTA',4X,'THETA1',4X,'THETA2',7X,'NSL',8X,'WF',      AL        215
     2  7X,'SMD',5X,'VFUEL'/11X,'(M)',7X,'(M)',6X,'(M-R)',4X,'(RAD)',       AL        216
     3  5X,'(RAD)',5X,'(RAD)',5X,'(RAD)',5X,'(RAD)',8X,'-',6X,'(KG/S)',     AL        217
     4  3X,'(MICRON)',2X,'(M/S)')                                          AL        218
      DO 818 I=1,NFNZ                                                       AL        219
      RNSL=FLOAT(NSL(I))                                                    AL        220
  818 WRITE (6,819) XO(I),YO(I),ZO(I),ALFA(I),BETA(I),DELTA(I),             AL        221
     1  THETA1(I),THETA2(I),RNSL,WFF(I),SMD(I),VFUEL(I)                    AL        222
  819 FORMAT (9X,1P12E10.2)                                                 AL        223
  813 CONTINUE                                                              AL        224
      WRITE (6,2037) FUTOT,AMASS,FUARAT                                     AL        225
 2037 FORMAT (/2X,'IV.   AIR-FUEL BALANCE'/8X,16(1H-)/                      AL        226
     1  30X,'TOTAL FUEL FLOW RATE----------',1PE12.4,'  (KG/S)'/           AL        227
     2  30X,'TOTAL AIR FLOW RATE-----------',1PE12.4,'  (KG/S)'/           AL        228
     3  30X,'FUEL TO AIR RATIO-------------',1PE12.4,/)                    AL        229
      WRITE (6,2040) CP,ARCON1,PREXP1,CR1,ARCON2,PREXP2,CR2,                AL        230
     1 C1,C2,CD                                                           $OUT       49
 2040 FORMAT (2X,'V.    SOME IMPORTANT QUANTITIES'/8X,24(1H-)/              AL        232
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     1  30X,'SPECIFIC HEAT--------------------',1PE12.4,'  (J/KG-K)'/      AL        233
     2  30X,'ACTIVATION ENERGY (1ST) ---------',1PE12.4,'  (K)'/           AL        234
     3  30X,'PRE-EXPONENT (1ST) --------------',1PE12.4,/                 AL        235
     3  30X,'EDDY BREAKUP CONSTANT (1ST) -----',1PE12.4,/                 AL        236
     7  30X,'ACTIVATION ENERGY (2ND) ---------',1PE12.4,'  (K)'/          AL        237
     8  30X,'PRE-EXPONENT (2ND) --------------',1PE12.4,/                 AL        238
     9  30X,'EDDY BREAKUP CONSTANT (2ND) -----',1PE12.4,/                 AL        239
     4  30X,'TURB. CONSTANT (C1) -------------',1PE12.4,/                 AL        240
     4  30X,'TURB. CONSTANT (C2) -------------',1PE12.4,/                 AL        241
     4  30X,'TURB. CONSTANT (CD) -------------',1PE12.4,/)                SOOT       50
      WRITE(6,2062)PREXP3,ARCON3,CR3,PREXP4,ARCON4,CR4                    4STEP      55
2062 FORMAT(30X,'PRE-EXPONENT (3RD) --------------',1PE12.4/              4STEP      56
     1       30X,'ACTIVATION ENERGY (3RD) ---------',1PE12.4/             4STEP      57
     1       30X,'EDDY BREAKUP CONSTANT (3RD) -----',1PE12.4/             4STEP      58
     1       30X,'PRE-EXPONENT (4TH) --------------',1PE12.4/             4STEP      59
     1       30X,'ACTIVATION ENERGY (4TH) ---------',1PE12.4/             4STEP      60
     1       30X,'EDDY BREAKUP CONSTANT (4TH) -----',1PE12.4)             4STEP      61
      WRITE(6,2064)AA1,BB1,CC1,AA2,BB2,CC2,AA3,BB3,CC3,AA4,BB4,CC4        4STEP      62
2064 FORMAT(30X,'SPECIES EXPONENTS,A,B,C(1ST) ---',1P3E12.4/              4STEP      63
     1 30X,'SPECIES EXPONENTS,A,B,C(2ND) ---',1P3E12.4/                  4STEP      64
     1 30X,'SPECIES EXPONENTS,A,B,C(3RD) ---',1P3E12.4/                  4STEP      65
     1 30X,'SPECIES EXPONENTS,A,B,C(4TH) ---',1P3E12.4)                  4STEP      66
C-----UNIT CONVERSION FOR 4-STEP RATE CONSTANTS.                         COMMENT    17
      PREXP1=PREXP1*(WFU**(1.0-AA1))/((WOX**BB1)*(WC2H4**CC1))           4STEP      67
     1*(10.0**(-3.0*(AA1+BB1+CC1)))                                      4STEP      68
      PREXP2=PREXP2*(WC2H4**(1.0-AA2))/((WOX**BB2)*(WFU**CC2))           4STEP      69
     1*(10.0**(-3.0*(AA2+BB2+CC2)))                                      4STEP      70
      PREXP3=PREXP3*(WCO**(1.0-AA3))/((WOX**BB3)*(WH2O**CC3))            4STEP      71
     1*(10.0**(-3.0*(AA3+BB3+CC3)))                                      4STEP      72
      PREXP4=PREXP4*(WH2**(1.0-AA4))/((WOX**BB4)*(WC2H4**CC4))           4STEP      73
     1*(10.0**(-3.0*(AA4+BB4+CC4)))                                      4STEP      74
      PEXP1=ALOG(PREXP1*(WFU**(AA1-1.0))*(WOX**BB1)*(WCH**CC1))          4STEP      75
      PEXP2=ALOG(PREXP2*(WCH**(AA2-1.0))*(WOX**BB2)*(WFU**CC2))          4STEP      76
      PEXP3=ALOG(PREXP3*(WCO**(AA3-1.0))*(WOX**BB3)*(WH2O**CC3))         4STEP      77
      PEXP4=ALOG(PREXP4*(WH2**(AA4-1.0))*(WOX**BB4)*(WCH**CC4))          4STEP      78
      ER1=ARCON1                                                         4STEP      79
      ER2=ARCON2                                                         4STEP      80
      ER3=ARCON3                                                         4STEP      81
      ER4=ARCON4                                                         4STEP      82
      CFRU1=CR1                                                          4STEP      83
      CERU2=CR2                                                          4STEP      84
      CERU3=CR3                                                          4STEP      85
      CERU4=CR4                                                          4STEP      86
      AEXP1=AA1                                                          4STEP      87
      AEXP2=AA2                                                          4STEP      88
      AEXP3=AA3                                                          4STEP      89
      AEXP4=AA4                                                          4STEP      90
      BEXP1=BB1                                                          4STEP      91
      BEXP2=BB2                                                          4STEP      92
      BEXP3=BB3                                                          4STEP      93
      BEXP4=BB4                                                          4STEP      94
      CEXP1=CC1                                                          4STEP      95
      CEXP2=CC2                                                          4STEP      96
      CEXP3=CC3                                                          4STEP      97
      CEXP4=CC4                                                          4STEP      98
      FST=FSTOIC                                                         4STEP      99
      IF(ITRAD.EQ.2)WRITE(6,2041)ABSOR,SCATR                             SOOT       51
 2041 FORMAT(                                                            SOOT       52
     5  30X,'ABSORPTION COEFFICIENT----------',1PE12.4,/                 AL        243
     6  30X,'SCATTERING COEFFICIENT----------',1PE12.4,/)                AL        244
      IF(ITRAD.EQ.3)WRITE(6,2043)                                        SOOT       53
 2043 FORMAT(30X,'ABSORPTION AND SCATTERING COEFFICIENTS CALCULATED'/)    SOOT       54
      IF(NSOOT.EQ.0)GO TO 401                                            SOOT       55
      WRITE(6,2045)(DPART(I),I=1,NPART)                                  SOOT       56
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 2045 FORMAT(30X,*SOOT PARTICLE DIAMETERS(MICRONS)*,1P5E12.4,/)          SOOT      57
      WRITE(6,2047)(FRACP(I),I=1,MPART)                                 SOOT      58
 2047 FORMAT(30X,*RELATIVE FORMATION RATES --------*,1P5E12.4,/)         SOOT      59
      DO 2049 II=1,MPART                                                SOOT      60
      DPART(II)=1.0E-6*DPART(II)                                        SOOT      61
 2049 FRACP(II)=0.01*FRACP(II)                                          SOOT      62
      WRITE(6,2054)AO,ARCONN,PREXPS,ARCOMS,ALPHA,AAS,BBS,AAA,BBB,FMG,   SOOT      63
     1 GO,RHCP                                                          SOOT      64
 2054 FORMAT(30X,*PRE-EXPONENT (NUCLEI) ----------*,1PE12.4,/           SOOT      65
     1        30X,*ACTIVATION ENERGY (NUCLEI) -----*,1PE12.4,/          SOOT      66
     2        30X,*PRE-EXPONENT (SOOT) ------------*,1PE12.4,/          SOOT      67
     3        30X,*ACTIVATION ENERGY (SOOT) -------*,1PE12.4,/          SOOT      68
     4        30X,*TEMPERATURE EXPONENT (SOOT) ----*,1PE12.4,/          SOOT      69
     5        30X,*FUEL EXPONENT (SOOT) -----------*,1PE12.4,/          SOOT      70
     6        30X,*OXYGEN EXPONENT (SOOT) ---------*,1PE12.4,/          SOOT      71
     7        30X,*CONSTANTS IN SOOT FORMATION -*,/                     SOOT      72
     8        35X,*A = *,1PE12.4,5X,*B = *,1PE12.4,/                    SOOT      73
     9        30X,*CONSTANTS IN NUCLEI FORMATION -*,/                   SOOT      74
     1        35X,*F-G = *,1PE12.4,5X,*GO = *,1PE12.4,/                 SOOT      75
     2        30X,*PARTICLE DENSITY ---------------*,1PE12.4,*  KG/M3*,/) SOOT      76
      WRITE(6,402)ISOOT,SSOOT,CINCP,TINCP                               SOOT      77
  402 FORMAT(30X,*SOOT CALCULATION STARTED AFTER ISTEP.GE.*,I3,          SOOT      78
     1 * OR SSUM.LE.*,1PE8.2/30X,*SOOT CALCULATION BYPASSED IF C/O RATIO SOOT      79
     1 LT.*,1PE8.2,* OR IF TEMPERATURE LT.*,1PE8.2)                     SOOT      80
  401 CONTINUE                                                          SOOT      81
      IF(IRAD.NE.1)WRITE(6,365)IRAD,SRAD                                SOOT      82
  365 FORMAT(30X,*RADIATION INCLUDED AFTER ISTEP.GE.*,I3,               SOOT      83
     1 * OR SSUM.LE.*,1PE8.2)                                           SOOT      84
      IF(NNOX.NE.0)WRITE(6,403)INOX,SNOX,TNOX                           NOX       82
  403 FORMAT(30X,*NOX CALCULATIONS STARTED AFTER ISTEP.GE.*,I3,          NOX       83
     1 * OR SSUM.LE.*,1PE8.2/30X,*NOX CALCULATION BYPASSED IF TEMPERATUR NOX       84
     1E LT.*,1PE8.2)                                                    NOX       85
      WRITE(6,2042)(RELAX(I),I=1,35)                                    4STEP     100
 2042 FORMAT (/8X,'RELAXATION PARAMETERS'/8X,21(1H-)/(5X,1P10E12.3))    AL        246
      GO TO (2050,2051), MODEL                                          AL        247
 2050 WRITE(6,2052)(PR(I),I=1,32)                                       4STEP     101
      GO TO 2053                                                        AL        249
 2051 WRITE(6,2052)(PREF(I),I=1,32)                                     4STEP     102
 2052 FORMAT (/8X,'PRANDTL NUMBERS'/8X,15(1H-)/(5X,1P10E12.3))          AL        251
 2053 CONTINUE                                                          AL        252
      WRITE (6,2044) (X(I),I=1,LP1)                                     AL        253
 2044 FORMAT (/8X,'X-COORDINATES'/8X,13(1H-)/(5X,1P10E12.3))            AL        254
      WRITE (6,2046) R(1),(Y(J),J=2,MP1)                                AL        255
 2046 FORMAT (/8X,'Y-COORDINATES'/8X,13(1H-)/(5X,1P10E12.3))            AL        256
      WRITE (6,2048) (Z(K),K=1,NP1)                                     AL        257
 2048 FORMAT (/8X,'Z-COORDINATES'/8X,13(1H-)/(5X,1P10E12.3))            AL        258
C +-+-+-+-+-+-+-+-+-+-+-+-+   CREATE INITIAL DATA TAPE   +-+-+-+-+-+-+-+-+-+-+-+- AL        259
C ---------   RESTART OPTIONS                                          AL        260
      IF (IRES.EQ.0) GO TO 201                                          AL        261
      REWIND NTP1                                                       AL        262
      DO 202 II=1,2                                                     AL        263
  202 READ (NTP1)                                                       AL        264
C -------- HERE PP IS PHI, P IS PFU, DU IS MCO                         AL        265
      READ (NTP1) PP,P,DU                                               AL        266
C -------- HERE DV IS ENTHALPY, DW IS FAV                              AL        267
      READ (NTP1) DV,DW                                                 AL        268
C-------- HERE U IS FX, V IS FY, W IS FZ                               AL        269
      READ (NTP1) U,V,W                                                 AL        270
      READ (NTP1) TEMP,RHO                                              AL        271
      READ(NTP1)FCH,FH2                                                 4STEP     103
      READ(NTP1)ANUC,SOOT1,SOOT2                                        SOOT      88
      READ(NTP1)FS                                                      NOX       89
C-----ABSORPTION AND SCATTERING COEFFICIENTS.                           COMMENT   10
      DO 203 K=1,NP1                                                    RAD       25
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      DO 203 J=1,MP1                                                    RAD       26
      DO 203 I=1,LP1                                                    RAD       27
      ABSR(I,J,K)=ABSOR                                                 RAD       28
  203 SCTR(I,J,K)=SCATR                                                 RAD       29
      RETURN                                                            AL       272
C ---------- ZERO ARRAYS                                                AL       273
  201 DO 204 NV=1,31                                                    4STEP    104
      DO 204 K=1,NP1                                                    AL       275
      DO 204 J=1,MP1                                                    AL       276
      KJM=KM(K)+JM(J)                                                   AL       277
      DO 204 I=1,LP1                                                    AL       278
      ABSR(I,J,K)=ABSOR                                                 RAD       30
      SCTR(I,J,K)=SCATR                                                 RAD       31
      LP=KJM+I                                                          AL       279
  204 F(LP,NV)=0.                                                       AL       280
      DO 205 K=2,N                                                      SOOT      90
      DO 205 J=2,M                                                      SOOT      91
      KJM=KM(K)+JM(J)                                                   SOOT      92
      DO 205 I=2,L                                                      SOOT      93
      LP=KJM+I                                                          SOOT      94
C------SPECIES CONCENTRATIONS.                                          COMMENT   19
      DO 207 INV=LVO2,LVOH                                              NOX       91
  207 F(LP,INV)=1.E-15                                                  NOX       92
      F(LP,NVS1)=1.E-5                                                  SOOT      95
      F(LP,NVS2)=1.E-6                                                  SOOT      96
  205 F(LP,NVN)=1.E8                                                    SOOT      97
C +-+-+-+-+-+-+-+-+-+-+-+-+-  U,V,W AND PRESSURE  -+-+-+-+-+-+-+-+-+-+-+-+-+ AL       281
      DO 451 K=1,NP1                                                    AL       282
      DO 451 J=2,M                                                      AL       283
      IS=IWLI(J,4)                                                      AL       284
      IE=IWLO(J,4)                                                      AL       285
      DO 451 I=IS,IE                                                    AL       286
      IF (I.EQ.IS) GO TO 452                                            AL       287
      U(I,J,K)=UIN(I)                                                   AL       288
  452 V(I,J,K)=0.0                                                      SOOT      98
      IF (J.EQ.JWLI(I,4)+1) GO TO 451                                   AL       290
      V(I,J,K)=0.0                                                      SOOT      99
  451 CONTINUE                                                          AL       292
      IF (IPAR.EQ.2) GO TO 255                                          AL       293
      DO 209 K=1,NP1                                                    AL       294
      DO 209 J=1,MP1                                                    AL       295
      IS=IWLI(J,5)                                                      AL       296
      IE=IWLO(J,5)                                                      AL       297
      DO 209 I=IS,IE                                                    AL       298
  209 P(I,J,K)=PRESS                                                    AL       299
C -------- BOUNDRY NODES                                               AL       300
  255 DO 240 K=1,NP1                                                    AL       301
      IF (IDW.EQ.1) GO TO 241                                           AL       302
      DO 242 I=3,LP1                                                    AL       303
      J=JWLI(I,4)                                                       AL       304
      U(I,J,K)=UIN(I)                                                   AL       305
  242 CONTINUE                                                          AL       306
  241 CONTINUE                                                          AL       307
      DO 244 J=JSW1,JSW2                                                AL       308
      I=IWLI(J,4)-1                                                     AL       309
      U(I+1,J,K)=USW                                                    AL       310
      V(I,J,K)=VSW                                                      AL       311
  244 V(I,J+1,K)=VSW                                                    AL       312
  247 CONTINUE                                                          AL       313
      DO 245 J=1,MP1                                                    AL       314
      I=IWLO(J,4)+1                                                     AL       315
      IF (J.LE.JWO1.OR.J.GE.JWO0) GO TO 245                             AL       316
      U(I,J,K)=U(I-1,J,K)                                               AL       317
  245 CONTINUE                                                          AL       318
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C -------- INJECTION POINTS                                              AL        319
C------FILM COOLING SLOTS.                                               COMMENT    20
      IF (NUINJ.LE.0) GO TO 240                                          AL        320
      DO 246 II=1,NUINJ                                                  AL        321
      I=IUINJ(II)                                                        AL        322
      J=JUINJ(II)                                                        AL        323
      U(I,J,K)=UINJ(II)                                                  AL        324
      U(I-1,J,K)=0.                                                      AL        325
  245 W(I-1,J,K)=WUINJ(II)                                               AL        326
  240 CONTINUE                                                           AL        327
C------DILUTION JETS.                                                   COMMENT    21
      IF (NVINJ.LE.0) GO TO 249                                          AL        328
      DO 250 II=1,NVINJ                                                  AL        329
      I=IVINJ(II)                                                        AL        330
      J=JVINJ(II)                                                        AL        331
      K=KVINJ(II)                                                        AL        332
      V(I,J,K)=VINJ(II)                                                  AL        333
      IF (J.EQ.JWLI(I,4)) V(I,J+1,K)=VINJ(II)                            AL        334
  250 CONTINUE                                                           AL        335
  249 CONTINUE                                                           AL        336
      REWIND NTP1                                                        AL        337
      WRITE (NTP1) U,V,W,P                                               AL        338
C +-+-+-+-+-+-+-+-  TURBULENT KINETIC ENERGY AND DISSIPATION  -+-+-+-+-+-+-+ AL        339
      DO 437 K=1,NP1                                                     AL        340
      DO 410 J=1,MP1                                                     AL        341
      KJM=KM(K)+JM(J)                                                    AL        342
      IS=IWLI(J,5)                                                       AL        343
      IE=IWLO(J,5)                                                       AL        344
      DO 410 I=IS,IE                                                     AL        345
      LP=KJM+I                                                           AL        346
      F(LP,NVK)=FK                                                       AL        347
      DY=Y(JWLO(I,4))-Y(J)                                               AL        348
      IF (IOW.EQ.1) DY=AMIN1(Y(JWLO(I,4))-Y(J),Y(J)-Y(JWLI(I,4)))        AL        349
      DY=AMAX1(DY,0.)                                                    AL        350
      AL=ALFAC*DY                                                        AL        351
  410 F(LP,NVD)=CD*FK**1.5/(AL+1.E-30)                                   AL        352
      DO 775 J=JSW1,JSW2                                                 AL        353
      LP=KM(K)+JM(J)+IWLI(J,4)-1                                         AL        354
  775 F(LP,NVD)=CD*FK**1.5/ALIN                                          AL        355
C------INJECTION POINTS.                                               COMMENT    22
C------FILM COOLING SLOTS.                                              COMMENT    23
      IF (NUINJ.LE.0) GO TO 437                                          AL        356
      DO 270 II=1,NUINJ                                                  AL        357
      I=IUINJ(II)-1                                                      AL        358
      J=JUINJ(II)                                                        AL        359
      LP=KM(K)+JM(J)+I                                                   AL        360
      F(LP,NVK)=AKFAC*(UINJ(II)**2+WUINJ(II)**2)                         AL        361
      AL=ALFAC*YS(J)                                                     AL        362
  270 F(LP,NVD)=CD*F(LP,NVK)**1.5/(AL+1.E-30)                            AL        363
  437 CONTINUE                                                           AL        364
C------DILUTION JETS.                                                   COMMENT    24
      IF (NVINJ.LE.0) GO TO 272                                          AL        365
      DO 274 II=1,NVINJ                                                  AL        366
      I=IVINJ(II)                                                        AL        367
      J=JVINJ(II)                                                        AL        368
      K=KVINJ(II)                                                        AL        369
      LP=KM(K)+JM(J)+I                                                   AL        370
      F(LP,NVK)=EVINJ(II)                                                AL        371
  274 F(LP,NVD)=CD*F(LP,NVK)**1.5/(DVINJ(II)+1.E-30)                     AL        372
  272 CONTINUE                                                           AL        373
C -------- HERE PP IS KE, P IS DISSIPATION                              AL        374
      WRITE (NTP1) PP,P                                                  AL        375
C +-+-+-+-+-+-+-+-+-+-+-+-+- PHI,FUEL,CO AND TEMP -+-+-+-+-+-+-+-+-+-+-+-+ AL        376
      DO 404 K=1,NP1                                                     AL        377
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      DO 404 J=1,MP1                                                    AL      378
      KJM=KM(K)+JM(J)                                                   AL      379
      IS=IWLI(J,5)                                                      AL      380
      IE=IWLO(J,5)                                                      AL      381
      DO 406 I=IS,IE                                                    AL      382
      LP=KJM+I                                                          AL      383
  406 F(LP,NVTE)=TIN(I)                                                 AL      384
      IS=IWLI(J,4)                                                      AL      385
      IE=IWLO(J,4)                                                      AL      386
      DO 404 I=IS,IE                                                    AL      387
      LP=KJM+I                                                          AL      388
      F(LP,NVFUDX)=FUDX(I)                                              AL      389
      F(LP,NVFU)=AMAX1(0.,F(LP,NVFUDX)-RATIO2*(1.-F(LP,NVFUDX))/RATIO1) AL      390
      F(LP,NVCH)=FUPCO                                                  4STEP   105
      F(LP,NVH2)=FUPCO                                                  4STEP   106
  404 F(LP,NVCC)=FUPCO                                                  AL      391
C -----BOUNDRY NODES                                                    AL      392
      DO 495 K=1,NP1                                                    AL      393
      DO 206 I=1,LP1                                                    AL      394
      J=JWLI(I,4)                                                       AL      395
      LP=KM(K)+JM(J)+I                                                  AL      396
      IF (IDW.EQ.0) GO TO 217                                           AL      397
      TEMP(I,J,K)=TCYLW                                                 AL      398
      IF (J.EQ.1) GO TO 208                                             AL      399
      TEMP(I,J,K)=TINLW                                                 AL      400
  208 F(LP,NVFUDX)=0.                                                   AL      401
      F(LP,NVFU)=0.                                                     AL      402
      F(LP,NVCO)=0.                                                     AL      403
      F(LP,NVCH)=0.0                                                    4STEP   107
      F(LP,NVH2)=0.0                                                    4STEP   108
      GO TO 216                                                         AL      404
  217 TEMP(I,J,K)=TIN(I)                                                AL      405
      F(LP,NVFUDX)=FUDX(I)                                              AL      406
      FEXIT=FUDX(I)-RATIO2*(1.-FUDX(I))/RATIO1                          AL      407
      F(LP,NVFU)=AMAX1(FEXIT,0.)                                        AL      408
      F(LP,NVCO)=0.                                                     AL      409
      F(LP,NVCH)=0.0                                                    4STEP   109
      F(LP,NVH2)=0.0                                                    4STEP   110
  216 J=JWLO(I,4)                                                       AL      410
      LP=KM(K)+JM(J)+I                                                  AL      411
      TEMP(I,J,K)=TCYLW                                                 AL      412
      IF (J.EQ.MP1) GO TO 444                                           AL      413
      TEMP(I,J,K)=TINLW                                                 AL      414
  444 F(LP,NVFU)=0.                                                     AL      415
      F(LP,NVCO)=0.                                                     AL      416
      F(LP,NVCH)=0.0                                                    4STEP   111
      F(LP,NVH2)=0.0                                                    4STEP   112
  206 F(LP,NVFUDX)=0.                                                   AL      417
      DO 210 J=1,MP1                                                    AL      418
      I=IWLT(J,4)-1                                                     AL      419
      LP=KM(K)+JM(J)+I                                                  AL      420
      IF (J.GE.JSW1.AND.J.LE.JSW2) GO TO 212                            AL      421
      TEMP(I,J,K)=TINLW                                                 AL      422
      F(LP,NVFUDX)=0.                                                   AL      423
      F(LP,NVFU)=0.                                                     AL      424
      F(LP,NVCO)=0.                                                     AL      425
      F(LP,NVCH)=0.0                                                    4STEP   113
      F(LP,NVH2)=0.0                                                    4STEP   114
      GO TO 213                                                         AL      426
  212 TEMP(I,J,K)=TSW                                                   AL      427
      F(LP,NVFUDX)=FUDXSW                                               AL      428
      F(LP,NVFU)=FUMSW                                                  AL      429
      F(LP,NVCO)=0.                                                     AL      430
      F(LP,NVCH)=0.0                                                    4STEP   115
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      F(LP,NVH2)=0.0                                                                    4STEP    116
  213 I=IWLO(J,4)+1                                                                     AL       431
      LP=KM(K)+JM(J)+I                                                                  AL       432
      IF (J.GT.JWOI.AND.J.LT.JWOO) GO TO 214                                            AL       433
      TEMP(I,J,K)=TINLW                                                                 AL       434
      F(LP,NVFUOX)=0.                                                                   AL       435
      F(LP,NVFU)=0.                                                                     AL       436
      F(LP,NVCO)=0.                                                                     AL       437
      F(LP,NVCH)=0.0                                                                    4STEP    117
      F(LP,NVH2)=0.0                                                                    4STEP    118
      GO TO 210                                                                         AL       438
  214 F(LP,NVFUOX)=FUOX(LP1)                                                            AL       439
      FEXIT=FUOX(LP1)-RATIO2*(1.-FUOX(LP1))/RATIO1                                      AL       440
      F(LP,NVFU)=AMAX1(FEXIT,0.)                                                        AL       441
      F(LP,NVTE)=TIN(I)                                                                 AL       442
      F(LP,NVCO)=0.                                                                     AL       443
      F(LP,NVCH)=0.0                                                                    4STEP    119
      F(LP,NVH2)=0.0                                                                    4STEP    120
  210 CONTINUE                                                                          AL       444
C -----INJECTION POINTS                                                               AL       445
C------FILM COOLING SLOTS.                                                            COMMENT   25
      IF (NUINJ.LE.0) GO TO 495                                                         AL       446
      DO 218 II=1,NUINJ                                                                 AL       447
      I=IUINJ(II)-1                                                                     AL       448
      J=JUINJ(II)                                                                       AL       449
      LP=KM(K)+JM(J)+I                                                                  AL       450
      F(LP,NVFUOX)=0.                                                                   AL       451
      F(LP,NVFU)=0.                                                                     AL       452
      F(LP,NVCO)=0.                                                                     AL       453
      F(LP,NVCH)=0.0                                                                    4STEP    121
      F(LP,NVH2)=0.0                                                                    4STEP    122
  218 TEMP(I,J,K)=TUINJ(II)                                                             AL       454
  495 CONTINUE                                                                          AL       455
C------DILUTION JETS.                                                                 COMMENT   26
      IF (NVINJ.LE.0) GO TO 220                                                         AL       456
      DO 222 II=1,NVINJ                                                                 AL       457
      I=IVINJ(II)                                                                       AL       458
      J=JVINJ(II)                                                                       AL       459
      K=KVINJ(II)                                                                       AL       460
      LP=KM(K)+JM(J)+I                                                                  AL       461
      F(LP,NVFUOX)=0.                                                                   AL       462
      F(LP,NVFU)=0.                                                                     AL       463
      F(LP,NVCO)=0.                                                                     AL       464
      F(LP,NVCH)=0.0                                                                    4STEP    123
      F(LP,NVH2)=0.0                                                                    4STEP    124
  222 TEMP(I,J,K)=TVINJ(II)                                                             AL       465
  220 CONTINUE                                                                          AL       466
C ---------- HERE PP IS PHI, P IS MFU AND DU IS MCO                                    AL       467
      WRITE (NTP1) PP,P,DU                                                              AL       468
C +-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+  ENTHALPY  +-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+   AL       469
      DO 276 K=1,NP1                                                                    AL       470
      DO 276 J=1,NP1                                                                    AL       471
      IS=IWLI(J,5)                                                                      AL       472
      IE=IWLO(J,5)                                                                      AL       473
      KJM=KM(K)+JM(J)                                                                   AL       474
      DO 276 I=IS,IE                                                                    AL       475
      LP=KJM+I                                                                          AL       476
      T=TEMP(I,J,K)                                                                     AL       477
      FUR=F(LP,NVFUOX)-F(LP,NVFU)                                                       AL       478
      FLPOX=RATIO1*F(LP,NVFU)+RATIO3*F(LP,NVCO)+RATIO2-(RATIO1+RATIO2)*                 AL       479
     1 F(LP,NVFUOX)+RATIO5*F(LP,NVCH)+RATIO6*F(LP,NVH2)                                 4STEP    125
      FLPOX=AMAX1(FLPOX,0.)                                                             AL       481
      FLPH2O=0.5*WH2O*(HYY*FUR/WFU-RATIO7*F(LP,NVCH)-F(LP,NVH2))                        4STEP    126
      FLPCO2=WCO2*(CXX*FUR/WFU-CXX*F(LP,NVCH)/WCH-F(LP,NVCO)/WCO)                       4STEP    127
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      FLPN2=1.-F(LP,NVFU)-FLPCO2-F(LP,NVCO)-FLPOX-FLPH2O                 AL      484
     1-F(LP,NVCH)-F(LP,NVH2)                                            4STEP   128
      IHCPS=3                                                           NOX      93
      NS1=IDFU                                                          NOX      94
      NS2=IDCO2                                                         NOX      95
      TK=T                                                              NOX      96
      TKINV=1.000/TK                                                    NOX      97
      FS(LP,IDFU)=F(LP,NVFU)                                            NOX      98
      FS(LP,IDO2)=FLPOX                                                 NOX      99
      FS(LP,IDN2)=FLPN2                                                 NOX     100
      FS(LP,IDCO)=F(LP,NVCO)                                            NOX     101
      FS(LP,IDCH)=F(LP,NVCH)                                            4STEP   129
      FS(LP,IDH2)=F(LP,NVH2)                                            4STEP   130
      FS(LP,IDH2O)=FLPH2O                                               NOX     102
      FS(LP,IDCO2)=FLPCO2                                               NOX     103
      DO 277 II=NS1,NS2                                                 NOX     104
  277 S2(II)=FS(LP,II)/SNW(II)                                          NOX     105
      CALL HCPS                                                         NOX     106
      HPI=HSUM*UNIICON*TK                                               NOX     107
      F(LP,NVH)=HPI                                                     AL      487
  276 CONTINUE                                                          AL      488
C +-+-+-+-+-+-+-+-+-+-+-+-+-+-  FX,FY,FZ AND FAV  -+-+-+-+-+-+-+-+-+-+-+ AL      489
      DO 791 K=1,NPJ                                                    AL      490
      DO 791 J=1,NPI                                                    AL      491
      KJM=KM(K)+JP(J)                                                   AL      492
      IS=IWLI(J,5)                                                      AL      493
      IE=IWLO(J,5)                                                      AL      494
      DO 791 I=IS,IE                                                    AL      495
      LP=KJM+I                                                          AL      496
      ST4=SIGMA*TEMP(I,J,K)**4                                          AL      497
      F(LP,NVRX)=ST4                                                    AL      498
      F(LP,NVRY)=ST4                                                    AL      499
      F(LP,NVRZ)=ST4                                                    AL      500
  791 F(LP,NVFAV)=ST4                                                   AL      501
C -------- HERE DV IS ENTHALPY, DW IS FAV                              AL      502
      WRITE (NTP1) DV,DW                                                AL      503
C -------- HERE U IS FX, V IS FY, W IS FZ                              AL      504
      WRITE (NTP1) U,V,W                                                AL      505
      WRITE(NTP1)TEMP,RHO                                               SOOT    100
C------$PECIES AND SOOT CONCENTRATIONS.                                 COMMENT  27
      WRITE(NTP1)FCH,FH2                                                4STEP   131
      WRITE(NTP1)ANUC,SOOT1,SOOT2                                       SOOT    101
      WRITE(NTP1)FS                                                     NOX     108
      RETURN                                                            AL      506
      END                                                               AL      507
      SUBROUTINE ALLMOD                                                 AL      508
      COMMON F(500,7),DU(10,10,5),DV(10,10,5),DW(10,10,5),              CONFA     2
     1 ANUC(10,10,5),SOOT1(10,10,5),SOOT2(10,10,5),FCH(10,10,5),        4STEP     1
     2 FH2(10,10,5),FS(500,14),                                         4STEP     2
     1 RHO(10,10,5),VISC(10,10,5),ABSR(10,10,5),SCTR(10,10,5),          RAD       1
     1 SU(10,10),SP(10,10),DRHODP(10,10,5),                             RAD       2
     1  AXP(10,10),AXM(10,10),AYP(10,10),AYM(10,10),AZP(10,10),         CONFA     4
     2  AZM(10,10),CZ(10,10),CY(10),CZU(10,10),CYU(10),                 CONFA     5
     3  CZP(10,10),CYP(10),DIVG(10,10),NTP1,NTP2                        CONFA     6
     1,AXMK(192),AXPK(192),AYMK(192),AYPK(192),AZMK(192),AZPK(192),     CTDMA     1
     2 SUK(192),SPK(192)                                                CTDMA     2
      DIMENSION U(10,10,5),V(10,10,5),W(10,10,5),PP(10,10,5)            CONFA     7
      DIMENSION P(10,10,5),TEMP(10,10,5),GAM(10,10,5)                   CONFA     8
      EQUIVALENCE (F(1,1),U(1,1,1)),(F(1,2),V(1,1,1)),(F(1,3),W(1,1,1)) CONFA     9
      EQUIVALENCE (F(1,4),PP(1,1,1)),(F(1,5),P(1,1,1))                  CONFA    10
      EQUIVALENCE (F(1,6),TEMP(1,1,1)),(F(1,7),GAM(1,1,1))              CONFA    11
      COMMON/CYL/R(30),RM(30),RMV(30),YSR(30),YSVR(30),IPLAN            COMMON    2
      COMMON/GRID/X(40),Y(30),Z(30),XS(40),YS(30),ZS(30),XSU(40),       COMMON    3
     1  YSV(30),ZSW(30),XDIF(40),YDIF(30),ZDIF(30),FXP(40),FXM(40),     COMMON    4
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     2  FYP(30),FYM(30),FZP(30),FZM(30),DT,TIME                          COMMON      5
      COMMON                                                             NOX         2
     1/CINDEX/IDCO,IDFU,IDO2,IDN2,IDH2O,IDCO2,IDH1,IDH2,IDM1,IDMO,IDMO2  NOX         3
     1,IDO,IDCH,IMCPS,ILC,ILH,IMAT,ITER,JJJ,M1,M2,M3,MA,MGLOB,MGLOBP,    NOX         4
     2 NLM,NO,NSP,NS1,NS2,IDCH                                          4STEP       3
     3/CCHEMI/CPSUM,HSUM,FQ,PPLN,RGAS,RGASIN,SMINV,TKINV,TLN,LNRG       NOX         6
     4/CPARAM/ASUB(30,3),ENV,ER,HSUBO,NDEBUG,NS,PA,QQ,Q1,Q2,Q3,Q4,RHOPP, NOX         7
     4 SM,SMW(30),SMO,S1(30),S2(30),TK,LADIAB,LDEBUG,LEQUIL,LREACT,     NOX         8
     4 LENER,EDKIJ,LCONVG                                               NOX         9
      DOUBLE PRECISION CPSUM,ENV,ER,FQ,HSUBO,HSUM,PA,PPLN,QQ,Q1,Q2,Q3,  NOX        10
     1 Q4,RGAS,RGASIN,RHOPP,SM,SMINV,SMW,S1,S2,TK,TKINV,TLN,SMO         NOX        11
     2,FUT,FST                                                          4STEP       4
      COMMON/STEP4/PEXP1,PEXP2,PEXP3,PEXP4,ER1,ER2,ER3,ER4,CEBU1,CEBU2, 4STEP       5
     1 CEBU3,CEBU4,AEXP1,AEXP2,AEXP3,AEXP4,BEXP1,BEXP2,BEXP3,BEXP4,     4STEP       6
     2 CEXP1,CEXP2,CEXP3,CEXP4,FUT,FST                                  4STEP       7
      LOGICAL LADIAB,LCONVG,LDEBUG,LEQUIL,LNRG,LREACT,LENER             NOX        12
      COMMON/INT/L,P,N,LCV,MCV,NCV,LP1,MP1,NP1,NI,NJ,NK,NINJ,NINJNK,NV,  COMMON      6
     1 NNV,NGOTO,K,ISTR,JSTR,KSTR,NVN(35),KM(30),JM(30),ISTEP,          4STEP       8
     2 ISOLVE(32),IPRINT(33),TITLE(10,33),IXY,ISWP,JSWP,RELAX(35),NP,   4STEP       9
     3  NRHO,NGAM,IWLI(30,5),IWLO(30,5),JWLO(40,5),JWLI(40,5),IWALL,    COMMON      9
     4  IWFO,PM1,JWIT,JWIO,JWOI,JWOO,IDM,JKIN(30,30),IKIN(40,30),       COMMON     10
      COMMON/INDEX/IPAR,LPREF,ISTUN,INCOMP,ITRAD,NVRX,NVRY,NVRZ,JPLANE   COMMON     11
     1,PLAXM1,LVK,LVD,LVFUOX,LVFU,LVCO,LVH,LVRX,LVRY,LVRZ,NVF(32),      4STEP      10
     2  IJUMP,IRFS,TITLE2(20),IMAX,JMAX,KMAX,NVCO,FUNCO,NVH2O,NVCO2,     COMMON     13
     3 NVN2,NVCH,NVH2                                                   4STEP      11
      COMMON/CNOX/LVH1,LVH2,LVN1,LVNO,LVNO2,LVO,LVOH,LVH2O,LVN2,LVO2,    NOX        16
     1 LVCO2,LVFU1,LVCO1,NNOX,INOX,ITNOX,SNOX,TNOX                      NOX        17
      COMMON/THERM/NVH,NVFU,NVOX,NVFUOX,NVTE,MODEN,IOK,FSTOIC,HFU,CP,    COMMON     15
     1  GASCON,RHOCON,UNICON,PRESS,NVFAV,TCYLW,TINLW,TLIP,ACOEF(4),      COMMON     16
     2  T4,OFAC,WFU,WCO2,WCO,WOX,WH2O,WN2,HYY,CXX,RATIO1,RATIO2,         COMMON     17
     3  RATIO3,RATIO4,HCO,TAN,ITWALL                                     COMMON     18
      COMMON/CTOMA/KEND,ICTOMA(32)                                      4STEP      12
      COMMON/MIS/APU,DEN,SMAX,SSUM,LASTEP,HTCEXT,CFR,EMISW,EMISIN,      COMGEN      2
     1  EMISR,TOUT,RTCO,EMI,RADIN,RADSUR,FMA,FK,SOFK,                    COMGEN      3
     2  FKFU,FOFU,TFUEL,WFN7,FLO(40),TEMTM(40),W(40),FUEL(40),FUOX(40) ,  COMGEN      4
     2 UIN(40),TIN(40),FUELS(40),SEXIT,IGAM1(29),IGAM2(29)              4STEP      13
      COMMON/TURB/NVK,NVD,C1,C2,CD,AK,DUIDXJ(3,3),AKFAC,ALFAC,          COMGEN      6
     1 MODEL,PR(32),PREF(32),PJAY(32),E                                 4STEP      14
      COMMON/RAD/NVE,SIGMA,ABSOR,SCATR                                  COMGEN      8
      COMMON/REACT/ARCON1,PREXP1,CR1,ARCON2,PREXP2,CR2,MODER            COMGEN      9
      COMMON/DROPL/EVAP(192),NTP4,NFN2,XO(3),YO(3),ZO(3),ALFA(3),       COMGEN     10
     1  BETA(3),DELTA(3),THETA1(3),THETA2(3),NSL(3),WFF(3),CMD(3),       COMGEN     11
     2  VFUEL(3),RFUEL(3),EVSU(64),HEVAP                                 COMGEN     12
      COMMON/INJEC/FLOWIN,IUINJ(20),JUINJ(20),UINJ(20),WUINJ(20),       COMGEN     13
     1  AUINJ(20),TUINJ(20),IVINJ(20),JVINJ(20),KVINJ(20),VINJ(20),      COMGEN     14
     2  EVINJ(20),DVINJ(20),AVINJ(20),TVINJ(20),NUINJ,NVINJ,JSW1,JSW2,   COMGEN     15
     3  USW,VSW,AFSW,FSW,TSW,WSW,SMNO,RHOSN                              COMGEN     16
      COMMON/CSOOT/NVN,NVS1,NVS2,ISOOT,SSOOT,NSOOT,AO,ARCONN,AAA,BBB,FMG  SOOT        8
     1,GO,MPART,DPART(2),FRACP(2),RHOP,ARCONS,PREXPS,ALPHA,AAS,BBS,DHR   SOOT        9
     2,LVN,LVS1,LVS2,CINCP,TINCP,FUTOT                                  SOOT       10
      COMMON/CRAD/IRAD,SRAD                                             SOOT       11
      COMMON/CFOUR/PREXP3,ARCON3,CR3,PREXP4,ARCON4,CR4,AA1,BB1,CC1,     4STEP      15
     1 AA2,BB2,CC2,AA3,BB3,CC3,AA4,BB4,CC4,RATIO5,RATIO6,RATIO7,        4STEP      16
     2 RATIO8,RATIO9,RATO10,RATO11,RATO12,WCH,WH2,WC2H4,LVCH,LVCH1,LVH21 4STEP      17
C  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  * AL        512
      ENTRY FMOD                                                        AL        513
C-----ENTRY FMOD IS USED TO UPDATE BOUNDARY VALUES AND TO LIMIT         COMMENT    28
C     SPECIES MASS FRACTIONS TO LIE BETWEEN 0.0 AND 1.0.                COMMENT    29
      NVFF=NVF(NV)                                                      AL        514
      IF(NV.NE.LVN)GO TO 1210                                           SOOT      102
C-----NUCLEI CONCENTRATION.                                             COMMENT    30
      DO 1211 K=2,N                                                     SOOT      103
      DO 1211 J=2,M                                                     SOOT      104
      KJM=KM(K)+JM(J)                                                   SOOT      105
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      DO 1211 I=2,L                                                     SOOT      106
      LP=KJM+I                                                          SOOT      107
 1211 F(LP,NVFF)=AMAX1(F(LP,NVFF),1.0)                                  SOOT      108
 1210 IF(NV.LT.LVS1.OR.NV.GT.LVS2)GO TO 1310                            SOOT      109
C-----SOOT CONCENTRATION.                                               COMMENT    31
      DO 1311 K=2,N                                                     SOOT      110
      DO 1311 J=2,M                                                     SOOT      111
      KJM=KM(K)+JM(J)                                                   SOOT      112
      DO 1311 I=2,L                                                     SOOT      113
      LP=KJM+I                                                          SOOT      114
      F(LP,NVFF)=AMAX1(F(LP,NVFF),1.E-30)                               SOOT      115
 1311 F(LP,NVFF)=AMIN1(F(LP,NVFF),1.0)                                  SOOT      116
 1310 CONTINUE                                                          SOOT      117
C-----SYMMETRY AXIS UPDATING.                                           COMMENT    32
      IF(NV.EQ.2)GO TO 1044                                             NASAX      11
      DO 1005 J=1,MP1                                                   NASAX      12
      DO 1005 K=2,N                                                     NASAX      13
      LP=LP1+JM(J)+KM(K)                                                NASAX      14
      LPW=LP-1                                                          NASAX      15
 1005 F(LP,NVFF)=F(LPW,NVFF)                                            NASAX      16
      IF(IDW.NE.0)GO TO 1044                                            NASAX      17
      DO 1006 I=2,LP1                                                   NASAX      18
      DO 1006 K=2,N                                                     NASAX      19
      LP=I+KM(K)                                                        NASAX      20
      LPN=LP+JM(2)                                                      NASAX      21
 1006 F(LP,NVFF)=F(LPN,NVFF)                                            NASAX      22
C ---------------  CYCLIC BOUNDARY CONDITIONS  ----------------------   AL        515
 1044 DO 1002 J=1,MP1                                                   AL        516
      DO 1002 I=1,LP1                                                   AL        517
      LIJ=I+JM(J)                                                       AL        518
      LP2=I+JM(J)+KM(2)                                                 AL        519
      LPN=LIJ+KM(N)                                                     AL        520
      LPNP1=LIJ+KM(NP1)                                                 AL        521
      F(LIJ,NVFF)=F(LPN,NVFF)                                           AL        522
      F(LPNP1,NVFF)=F(LP2,NVFF)                                         AL        523
 1002 CONTINUE                                                          AL        524
 1001 CONTINUE                                                          AL        525
      IF(NV.NE.LVFUOX)GO TO 1010                                        4STEP     132
C-----MIXTURE FRACTION.                                                 COMMENT    33
      DO 1020 K=1,NP1                                                   AL        527
      DO 1020 J=1,MP1                                                   AL        528
      KJM=KM(K)+JM(J)                                                   AL        529
      DO 1020 I=1,LP1                                                   AL        530
      LP=KJM+I                                                          AL        531
      F(LP,NVFF)=AMAX1(F(LP,NVFF),0.)                                   AL        532
      F(LP,NVFF)=AMIN1(F(LP,NVFF),1.0)                                  4STEP     133
 1020 CONTINUE                                                          AL        534
      GO TO 1036                                                        4STEP     134
 1010 IF(NV.NE.LVFU)GO TO 1030                                          4STEP     135
C-----FUEL CONCENTRATION.                                               COMMENT    34
      DO 1031 K=1,NP1                                                   4STEP     136
      DO 1031 J=1,MP1                                                   4STEP     137
      KJM=KM(K)+JM(J)                                                   4STEP     138
      DO 1031 I=1,LP1                                                   4STEP     139
      LP=KJM+I                                                          4STEP     140
      F(LP,NVFF)=AMIN1(F(LP,NVFF),F(LP,NVFUOX))                         4STEP     141
 1031 F(LP,NVFF)=AMAX1(F(LP,NVFF),0.0)                                  4STEP     142
      GO TO 1036                                                        4STEP     143
 1030 IF(NV.NE.LVCH)GO TO 1032                                          4STEP     144
C-----INTERMEDIATE HYDROCARBON CONCENTRATION.                           COMMENT    35
      DO 1033 K=1,NP1                                                   4STEP     145
      DO 1033 J=1,MP1                                                   4STEP     146
      KJM=KM(K)+JM(J)                                                   4STEP     147
      DO 1033 I=1,LP1                                                   4STEP     148
```

```
      LP=KJM+I                                                          4STEP     149
      F(LP,NVFF)=AMIN1(F(LP,NVFF),RATIO8*(F(LP,NVFUOX)-F(LP,NVFU)))     4STEP     150
 1033 F(LP,NVFF)=AMAX1(F(LP,NVFF),1.0E-5)                               MAR2        1
      GO TO 1036                                                        4STEP     152
 1032 IF(NV.NE.LVGU)GO TO 1034                                          4STEP     153
C-----GU CONCENTRATION.                                                 COMMENT    36
      DO 1035 K=1,NP1                                                   4STEP     154
      DO 1035 J=1,MP1                                                   4STEP     155
      KJM=KM(K)+JM(J)                                                   4STEP     156
      DO 1035 I=1,LP1                                                   4STEP     157
      LP=KJM+I                                                          4STEP     158
      F(LP,NVFF)=AMIN1(F(LP,NVFF),RATIO4*(F(LP,NVFUOX)-F(LP,NVFU))      4STEP     159
     1-RATIO11*F(LP,NVCH))                                              4STEP     160
 1035 F(LP,NVFF)=AMAX1(F(LP,NVFF),1.0E-5)                               MAR2        2
      GO TO 1036                                                        4STEP     162
 1034 IF(NV.NE.LVH2)GO TO 1036                                          4STEP     163
C-----H2 CONCENTRATION.                                                 COMMENT    37
      DO 1037 K=1,NP1                                                   4STEP     164
      DO 1037 J=1,MP1                                                   4STEP     165
      KJM=KM(K)+JM(J)                                                   4STEP     166
      DO 1037 I=1,LP1                                                   4STEP     167
      LP=KJM+I                                                          4STEP     168
      F(LP,NVFF)=AMIN1(F(LP,NVFF),RATIO9*(F(LP,NVFUOX)-F(LP,NVFU))      4STEP     169
     1-RATO10*F(LP,NVCH))                                               4STEP     170
 1037 F(LP,NVFF)=AMAX1(F(LP,NVFF),1.0E-5)                               MAR2        3
 1036 CONTINUE                                                          4STEP     172
      RETURN                                                            AL        536
C  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  * AL        537
      ENTRY VELMOD                                                      AL        538
C-----ENTRY VELMOD IS USED FOR VELOCITY MODIFICATIONS.                  COMMENT    38
C                                                                       COMMENT    39
C-----INTRODUCE SWIRL GRADUALLY.                                        COMMENT    40
      DO 1000 K=1,NP1                                                   AL        539
      DO 1000 J=JSW1,JSW2                                               AL        540
      WIN=WSW*R(J)/R(JSW2)                                              AL        541
      I=IWLI(J,4)-1                                                     AL        542
      W(I,J,K)=W(I,J,K)+.02*WIN                                         AL        543
      IF (ABS(W(I,J,K)).GT.ABS(WIN)) W(I,J,K)=WIN                       AL        544
 1000 CONTINUE                                                          AL        545
 1003 CONTINUE                                                          AL        546
      DO 2005 J=2,M                                                     AL        547
      DO 2005 I=2,L                                                     AL        548
      W(I,J,2)=W(I,J,NP1)                                               AL        549
 2007 DW(I,J,2)=DW(I,J,NP1)                                             AL        550
 2005 CONTINUE                                                          AL        551
C  ------   SATISFY CONTINUITY AT EXIT PLANE                           AL        552
      RHOA=0.0                                                          AL        553
      FLOWOT=0.0                                                        AL        554
      INDX=0                                                            AL        555
      DO 755 K=2,N                                                      AL        556
      JS=JWLI(LP1,4)+1                                                  AL        557
      JE=JWLO(LP1,4)-1                                                  AL        558
      DO 755 J=JS,JE                                                    AL        559
      RHO(LP1,J,K)=RHO(L,J,K)                                           AL        560
      ROA=YSK(J)*ZS(K)*RHO(LP1,J,K)                                     AL        561
      RHOA=RHOA+ROA                                                     AL        562
      FLOWOT=FLOWOT+U(L,J,K)*ROA                                        AL        563
      IF (U(L,J,K).GE.0.0) GO TO 755                                    AL        564
      INDX=1                                                            AL        565
  755 CONTINUE                                                          AL        566
      UADD=(FLOWIN-FLOWOT)/RHOA                                         AL        567
      SEXIT=1.-FLOWOT/FLOWIN                                            AL        568
      UMEAN=FLOWIN/RHOA                                                 AL        569
      DO 756 K=2,N                                                      AL        570
```

```
      JS=JWLI(LP1,4)+1                                                  AL        571
      JE=JWLO(LP1,4)-1                                                  AL        572
      DO 756 J=JS,JE                                                    AL        573
      U(LP1,J,K)=AMAX1(0.0,U(L,J,K)+UADD)                               NASAX      21
  756 CONTINUE                                                          AL        574
      RETURN                                                            AL        575
C  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  * AL        576
      ENTRY DENMOD                                                      AL        577
C-----ENTRY DENMOD IS USED FOR MODIFYING DENSITIES AT RADIAL            COMMENT    41
C     INJECTION HOLES, INLET SWIRLER, AND FILM COOLING SLOTS.           COMMENT    42
C                                                                       COMMENT    43
      IF (NVINJ.LE.0) GO TO 750                                         AL        582
C-----RADIAL INJECTION.                                                 COMMENT    44
      DO 749 II=1,NVINJ                                                 AL        583
      I=IVINJ(II)                                                       AL        584
      K=KVINJ(II)                                                       AL        585
      J=JVINJ(II)                                                       AL        586
      M1=J                                                              AL        587
      IF (J.EQ.JWLI(I,4)) M1=J+1                                        AL        588
      AREA=XS(I)*RM(M1)*ZS(K)                                           AL        589
      RHOINJ=AVINJ(II)/ABS(VINJ(II))/AREA                               AL        590
  749 RHO(I,J,K)=RHOINJ                                                 AL        591
  750 CONTINUE                                                          AL        592
C-----CYCLIC BOUNDARY CONDITIONS.                                       COMMENT    45
      DO 2060 J=2,M                                                     AL        593
      DO 2060 I=2,L                                                     AL        594
      RHO(I,J,NP1)=.5*(RHO(I,J,2)+RHO(I,J,N))                           AL        595
      RHO(I,J,1)=RHO(I,J,NP1)                                           AL        596
2060  CONTINUE                                                          AL        597
C-----INLET SWIRLER.                                                    COMMENT    46
      DO 760 K=1,NP1                                                    AL        598
      DO 2061 J=JSW1,JSW2                                               AL        599
      I=IWLI(J,4)-1                                                     AL        600
 2061 RHO(I,J,K)=RHOSW                                                  AL        601
 2099 CONTINUE                                                          AL        602
C-----FILM COOLING SLOTS.                                               COMMENT    47
 2064 IF (NUINJ.LE.0) GO TO 760                                         AL        603
      DO 759 II=1,NUINJ                                                 AL        604
      I=IUINJ(II)-1                                                     AL        605
      J=JUINJ(II)                                                       AL        606
      AREA=YSR(J)*(Z(NP1)-Z(1))                                         AL        607
  759 RHO(I,J,K)=2.*AUINJ(II)/AREA/UINJ(II)-RHO(I+1,J,K)                AL        608
  760 CONTINUE                                                          AL        609
      RETURN                                                            AL        610
C  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  * AL        611
      ENTRY GAMOD                                                       AL        612
C-----ENTRY GAMOD IS USED TO CALCULATE WALL GAMAS FROM THE WALL         COMMENT    48
C     FUNCTIONS.                                                        COMMENT    49
C                                                                       COMMENT    50
      DO 3000 K=1,NP1                                                   AL        613
      DO 3007 I=1,LP1                                                   AL        614
      J=JWLO(I,4)                                                       AL        615
      IF (IKIN(I,K).EQ.2.OR.IKIN(I,K).EQ.3) GO TO 3003                  AL        616
      IF (IGAM1(NV).EQ.0) GO TO 3003                                    AL        617
      YPLUS=VISC(I,J,K)                                                 AL        618
      IF (YPLUS.GT.11.5) GO TO 3001                                     AL        619
      GAM(I,J,K)=AMU/PR(NV)                                             AL        620
      GO TO 3002                                                        AL        621
 3001 GAM(I,J,K)=AMU*YPLUS/PREF(NV)/(ALOG(E*YPLUS)/AK+PSAT(NV))         AL        622
      GO TO 3002                                                        AL        623
 3003 GAM(I,J,K)=0.                                                     AL        624
 3002 J=JWLI(I,4)                                                       AL        625
      IF (IOW.EQ.0.OR.IKIN(I,K).EQ.1.OR.IKIN(I,K).EQ.3) GO TO 3004      AL        626
      IF (IGAM1(NV).EQ.0) GO TO 3004                                    AL        627
```

```
      YPLUS=VISC(I,J,K)                                                  AL       628
      IF (YPLUS.GT.11.5) GO TO 3006                                      AL       629
      GAM(I,J,K)=AMU/PR(NV)                                              AL       630
      GO TO 3007                                                         AL       631
 3006 GAM(I,J,K)=AMU*YPLUS/PREF(NV)/(ALOG(E*YPLUS)/AK+PJAY(NV))          AL       632
      GO TO 3007                                                         AL       633
 3004 GAM(I,J,K)=0.                                                      AL       634
 3007 CONTINUE                                                           AL       635
      DO 3000 J=2,M                                                      AL       636
      I=IWLI(J,4)-1                                                      AL       637
      IF (JKIN(J,K).EQ.1) GO TO 3009                                     AL       638
      IF (IGAM2(NV).EQ.0) GO TO 3009                                     AL       639
      YPLUS=VISC(I,J,K)                                                  AL       640
      IF (YPLUS.GT.11.5) GO TO 3019                                      AL       641
      GAM(I,J,K)=AMU/PR(NV)                                              AL       642
      GO TO 3011                                                         AL       643
 3019 GAM(I,J,K)=AMU*YPLUS/PREF(NV)/(ALOG(E*YPLUS)/AK+PJAY(NV))          AL       644
      GO TO 3011                                                         AL       645
 3009 GAM(I,J,K)=0.                                                      AL       646
 3011 I=IWLO(J,4)+1                                                      AL       647
      IF (J.GT.JWCI.AND.J.LT.JW00) GO TO 3012                            AL       648
      IF (IGAM2(NV).EQ.0) GO TO 3012                                     AL       649
      YPLUS=VISC(I,J,K)                                                  AL       650
      IF (YPLUS.GT.11.5) GO TO 3013                                      AL       651
      GAM(I,J,K)=AMU/PR(NV)                                              AL       652
      GO TO 3000                                                         AL       653
 3013 GAM(I,J,K)=AMU*YPLUS/PREF(NV)/(ALOG(E*YPLUS)/AK+PJAY(NV))          AL       654
      GO TO 3000                                                         AL       655
 3012 GAM(I,J,K)=0.                                                      AL       656
 3000 CONTINUE                                                           AL       657
CYCLIC BOUNDARY CONDITIONS.                                             COMMENT    51
      DO 3014 I=2,L                                                      AL       658
      DO 3014 J=2,M                                                      AL       659
      GAM(I,J,1)=.5*(GAM(I,J,2)+GAM(I,J,N))                              AL       660
      GAM(I,J,NP1)=GAM(I,J,1)                                            AL       661
      IF (NV.EQ.3) GAM(I,J,NP1)=GAM(I,J,2)                               AL       662
 3014 CONTINUE                                                           AL       663
      RETURN                                                             AL       664
C **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  AL       665
      ENTRY SOMAS                                                        AL       666
C-----ENTRY SOMAS IS USED TO INCLUDE THE SPRAY EVAPORATION TERM          COMMENT    52
C     IN THE VARIOUS EQUATIONS.                                          COMMENT    53
C                                                                        COMMENT    54
      DO 124 I=1,LP1                                                     AL       667
      DO 124 J=1,MP1                                                     AL       668
  124 DIVG(I,J)=0.                                                       AL       669
      GO TO (266,267,268,269), NGOTO                                     AL       670
C ---------  U-VELOCITY                                                  AL       671
  266 CONTINUE                                                           AL       672
  270 IF (NFN2.LE.0) GO TO 271                                           AL       673
      DO 273 J=2,M                                                       AL       674
      KJK=(K-2)*(NI-2)*(NJ-2)+(J-2)*(NI-2)                               AL       675
      IS=IWLI(J,NGOTO)                                                   AL       676
      IE=IWLO(J,NGOTO)                                                   AL       677
      DO 273 I=IS,IE                                                     AL       678
      LPC=KJK+(I-1)                                                      AL       679
      LXMC=LPC-1                                                         AL       680
      DIVG(I,J)=DIVG(I,J)-FXM(I-1)*EVAP(LXMC)-FXP(I)*EVAP(LPC)           AL       681
      IF (I.EQ.3) DIVG(I,J)=DIVG(I,J)-FXP(2)*EVAP(LXMC)                  AL       682
      IF (I.EQ.L) DIVG(I,J)=DIVG(I,J)-FXM(L)*EVAP(LPC)                   AL       683
  273 CONTINUE                                                           AL       684
  271 CONTINUE                                                           AL       685
      RETURN                                                             AL       686
C ---------  V-VELOCITY                                                  AL       687
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  267 CONTINUE                                                          AL      688
  274 IF (NFN7.LE.0) GO TO 276                                          AL      689
      DO 277 J=3,M                                                      AL      690
      KJK=(K-2)*(NI-2)*(NJ-2)+(J-2)*(NI-2)                              AL      691
      IS=IWLI(J,NGOTO)                                                  AL      692
      IE=IWLO(J,NGOTO)                                                  AL      693
      DO 277 I=IS,IE                                                    AL      694
      LPC=KJK+(I-1)                                                     AL      695
      LYMC=LPC-(NI-2)                                                   AL      696
      DIVG(I,J)=DIVG(I,J)-FYM(J-1)*EVAP(LYMC)-FYP(J)*EVAP(LPC)          AL      697
      IF (J.EQ.3) DIVG(I,J)=DIVG(I,J)-FYP(2)*EVAP(LYMC)                 AL      698
      IF (J.EQ.M) DIVG(I,J)=DIVG(I,J)-FYM(M)*EVAP(LPC)                  AL      699
  277 CONTINUE                                                          AL      700
  276 CONTINUE                                                          AL      701
      RETURN                                                            AL      702
C ---------  W-VELOCITY                                                 AL      703
  268 CONTINUE                                                          AL      704
  278 IF (NFN7.LE.0) GO TO 281                                          AL      705
      DO 282 J=2,M                                                      AL      706
      KJK=(K-2)*(NI-2)*(NJ-2)+(J-2)*(NI-2)                              AL      707
      IS=IWLI(J,NGOTO)                                                  AL      708
      IE=IWLO(J,NGOTO)                                                  AL      709
      DO 282 I=IS,IE                                                    AL      710
      LPC=KJK+(I-1)                                                     AL      711
      LZMC=LPC-(NI-2)*(NJ-2)                                            AL      712
      LIJ=(J-2)*(NI-2)+(I-1)                                            AL      713
      DIVG(I,J)=DIVG(I,J)-FZM(K-1)*EVAP(LZMC)                           AL      714
      IF (K.LT.NP1) DIVG(I,J)=DIVG(I,J)-FZP(K)*EVAP(LPC)                AL      715
      IF (K.EQ.NP1) DIVG(I,J)=DIVG(I,J)-FZP(2)*EVAP(LIJ)                AL      716
  282 CONTINUE                                                          AL      717
  281 CONTINUF                                                          AL      718
      RETURN                                                            AL      719
C --------  OTHER VARIABLES                                            AL      720
  269 CONTINUF                                                          AL      721
  283 IF (NFN7.LE.0) GO TO 285                                          AL      722
      DO 286 J=2,M                                                      AL      723
      KJK=(K-2)*(NI-2)*(NJ-2)+(J-2)*(NI-2)                              AL      724
      IS=IWLI(J,NGOTO)                                                  AL      725
      IE=IWLO(J,NGOTO)                                                  AL      726
      DO 286 I=IS,IE                                                    AL      727
      LPC=KJK+(I-1)                                                     AL      728
      DIVG(I,J)=DIVG(I,J)-EVAP(LPC)                                     AL      729
  286 CONTINUE                                                          AL      730
  285 CONTINUE                                                          AL      731
      RETURN                                                            AL      732
C  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  * AL      733
      ENTRY SOMOD                                                       AL      734
C------ENTRY SOMOD IS USED TO INTRODUCE THE BOUNDARY CONDITIONS        COMMENT   55
C     BY MODIFYING THE SOURCE TERMS.                                    COMMENT   56
C                                                                       COMMENT   57
COME HERE FOR SLOT COEFFICIENT MODS.                                    AL      735
   54 IF (NUINJ.LE.0) GO TO 52                                          AL      736
      DO 49 II=1,NUINJ                                                  AL      737
      I=IUINJ(II)                                                       AL      738
      J=JUINJ(II)                                                       AL      739
      IF (J.EQ.JWLI(I,4)+1) GO TO 149                                   AL      740
      M1=J-1                                                            AL      741
      IF (NV.EQ.1) AYP(I,M1)=.5*AYP(I,M1)                               AL      742
      IF (NV.EQ.1) AYP(I-1,M1)=.5*AYP(I-1,M1)                           AL      743
      IF (NV.GT.2) AYP(I-1,M1)=0.                                       AL      744
      IF (NV.NE.1) AYP(I-2,J)=0.                                        AL      745
      IF (NV.EQ.LVRX) AXM(I,J)=0.                                       AL      746
      GO TO 49                                                          AL      747
  149 M1=J+1                                                            AL      748
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```
      IF (NV.EQ.1) AYM(I,M1)=.5*AYM(I,M1)                                AL        749
      IF (NV.EQ.1) AYM(I-1,M1)=.5*AYM(I-1,M1)                            AL        750
      IF (NV.GT.2) AYM(I-1,M1)=0.                                        AL        751
      IF (NV.NE.1) AXP(I-2,J)=0.                                         AL        752
      IF (NV.EQ.LVRX) AXM(I,J)=0.                                        AL        753
   49 CONTINUE                                                           AL        754
   99 CONTINUE                                                           AL        755
C +-+-+-+-+-+-+-+-+-+-+-+-   PRESSURE PERTABATION   +-+-+-+-+-+-+-+-+-+-+-+-+-+ AL  756
      IF(NV.NE.4) GO TO 200                                              AL        757
C-----SLOT MODIFICATIONS.                                                COMMENT    58
      IF (NUINJ.LE.0) GO TO 99                                           AL        758
      DO 98 II=1,NUINJ                                                   AL        759
      I=IUINJ(II)-1                                                      AL        760
      J=JUINJ(II)                                                        AL        761
      SU(I,J)=0.                                                         AL        762
   98 SP(I,J)=-1.E30                                                     AL        763
   99 CONTINUE                                                           AL        764
COME HERE FOR DROPLET EVAPORATION TERMS                                  AL        765
      IF (NFNZ.LE.0) GO TO 344                                           AL        766
      DO 346 J=2,N                                                       AL        767
      KJK=(K-2)*(NI-2)*(NJ-2)+(J-2)*(NI-2)                               AL        768
      IS=IWLI(J,NGOTO)                                                   AL        769
      IE=IWLO(J,NGOTO)                                                   AL        770
      DO 346 I=IS,IE                                                     AL        771
      LPC=KJK+(I-1)                                                      AL        772
  346 SU(I,J)=SU(I,J)+EVAP(LPC)                                          AL        773
  344 CONTINUE                                                           AL        774
C-----CALCULATE THE MAXIMUM AND SUM OF CONTINUITY ERRORS.                COMMENT    59
      IF(K.NE.2) GO TO 101                                               AL        775
      SMAX=0.                                                            AL        776
      SSUM=0.                                                            AL        777
  101 CONTINUE                                                           AL        778
      DO 100 J=2,N                                                       AL        779
      IS=IWLI(J,NGOTO)                                                   AL        780
      IE=IWLO(J,NGOTO)                                                   AL        781
      DO 100 I=IS,IE                                                     AL        782
      ASU=ABS(SU(I,J))                                                   AL        783
      SSUM=SSUM+ASU                                                      AL        784
      IF (ASU.LT.SMAX) GO TO 100                                         AL        785
      IMAX=I                                                             AL        786
      JMAX=J                                                             AL        787
      KMAX=K                                                             AL        788
      SMAX=ASU                                                           AL        789
  100 CONTINUE                                                           AL        790
      IF(K.NE.N) GO TO 102                                               AL        791
      SMAX=SMAX/FLOWIN                                                   AL        792
      SSUM=SSUM/FLOWIN                                                   AL        793
  102 CONTINUE                                                           AL        794
  200 CONTINUE                                                           AL        795
C +-+-+-+-+-+-+-+-+-+-+-+-   TURBULENCE DISSIPATION   +-+-+-+-+-+-+-+-+-+-+-+-+-+ AL  796
      IF (NV.NE.LVD) GO TO 300                                           AL        797
COME HERE FOR CYLINDRICAL WALL SOURCE TERMS                              AL        798
      DO 201 I=2,L                                                       AL        799
      J=JWLO(I,NGOTO)-1                                                  AL        800
      IF (IKIN(I,K).EQ.2.OR.IKIN(I,K).EQ.3) GO TO 1201                   AL        801
      DIST=.5*YDIF(J+1)                                                  AL        802
      IF (J.EQ.M) DIST=YDIF(MP1)                                         AL        803
      LP=KM(K)+JM(J)+I                                                   AL        804
      RTCOK=RTCOF(LP,NVK)                                                AL        805
      SU(I,J)=1.E30*RTCOK*SQRT(RTCOK)/(AK*DIST)                          AL        806
      SP(I,J)=-1.E30                                                     AL        807
 1201 IF (IDW) 201,201,1200                                              AL        808
 1200 J=JWLI(I,NGOTO)+1                                                  AL        809
      IF (IKIN(I,K).EQ.1.OR.IKIN(I,K).EQ.3) GO TO 201                    AL        810
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```
      DIST=.5*YDIF(J)
      IF (J.EQ.2) DIST=YDIF(2)
      LP=KM(K)+JM(J)+I
      RTCDK=RTCD*F(LP,NVK)
      SU(I,J)=1.E30*RTCDK*SQRT(RTCDK)/(AK*DIST)
      SP(I,J)=-1.E30
201   CONTINUE
COME HERE FOR SLOT MODIFICATIONS
      IF (NUINJ.LE.0) GO TO 710
      DO 709 II=1,NUINJ
      I=IUINJ(II)-1
      J=JUINJ(II)
      M1=J-1
      IF (J.EQ.JWLI(I,NGOTO)+1) M1=J+1
      M2=AMAXO(M1,J)
      LP=KM(K)+JM(M1)+I
      RTCDK=RTCD*F(LP,NVK)
      SKE=AKFAC*(UINJ(II)**2+WUINJ(II)**2)
      SLM=ALFAC*YS(J)
      SU(I,J)=1.E30*CD*SKE**1.5/(SLM+1.E-30)
      SP(I,J)=-1.E30
      SU(I,M1)=1.E30*RTCDK*SQRT(RTCDK)/(AK*.5*YDIF(M2))
      SP(I,M1)=-1.E30
  709 CONTINUE
  710 CONTINUE
COME HERE FOR INLET WALL SOURCE TERMS
      DO 202 J=2,MM1
      I=IWLI(J,NGOTO)
      IF (JKIN(J,K).EQ.1) GO TO 1202
      LP=I+JM(J)+KM(K)
      RTCDK=RTCD*F(LP,NVK)
      DIST=.5*XDIF(I)
      IF (I.EQ.2) DIST=XDIF(2)
      SU(I,J)=1.E30*RTCDK*SQRT(RTCDK)/(AK*DIST)
      SP(I,J)=-1.E30
 1202 I=IWLO(J,NGOTO)
      IF (J.GT.JWCI.AND.J.LT.JWOO) GO TO 202
      LP=I+JM(J)+KM(K)
      RTCDK=RTCD*F(LP,NVK)
      DIST=.5*XDIF(I+1)
      IF (I.EQ.L) DIST=XDIF(LP1)
      SU(I,J)=1.E30*RTCDK*SQRT(RTCDK)/(AK*DIST)
      SP(I,J)=-1.E30
202   CONTINUE
C +-+-+-+-+-+-+-+-+-+-+-   U-VELOCITY   +-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-
  300 IF (NV.NE.1) GO TO 400
COME HERE FOR SLOT MODIFICATIONS
      IF (NUINJ.LE.0) GO TO 720
      DO 719 II=1,NUINJ
      I=IUINJ(II)
      J=JUINJ(II)
      SU(I,J)=1.E30*UINJ(II)
      SP(I,J)=-1.E30
  719 SP(I-1,J)=-1.E30
  720 CONTINUE
COME HERE FOR DROPLET EVAPORATION TERMS
      IF (NFN7.LE.0) GO TO 321
      IF (K.EQ.2) REWIND NTP4
      READ (NTP4) EVSU
      DO 322 J=2,M
      KJK=(K-2)*(NI-2)*(NJ-2)+(J-2)*(NI-2)
      IS=IWLI(J,NGOTO)
      IE=IWLO(J,NGOTO)
      DO 322 I=IS,IE
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```
      LPC=KJK+(I-1)                                                          AL       875
      LXMC=LPC-1                                                             AL       876
      LIJ=(J-2)*(NI-2)+(I-1)                                                 AL       877
      SU(I,J)=SU(I,J)+EVSU(LIJ)                                              AL       878
      SP(I,J)=SP(I,J)-FXM(I-1)*EVAP(LXMC)-FXP(I)*EVAP(LPC)                   AL       879
      IF (I.EQ.3) SP(I,J)=SP(I,J)-FXP(2)*EVAP(LXMC)                          AL       880
      IF (I.EQ.L) SP(I,J)=SP(I,J)-FXM(L)*EVAP(LPC)                           AL       881
  322 CONTINUE                                                               AL       882
  321 CONTINUE                                                               AL       883
C +-+-+-+-+-+-+-+-+-+-+-+-+-+    W-VELOCITY    +-+-+-+-+-+-+-+-+-+-+-+-+-+ AL       884
400   IF(NV.NE.3) GO TO 500                                                  AL       885
COME HERE FOR SLOT MODIFICATIONS                                             AL       886
      IF (NUINJ.LE.0) GO TO 502                                              AL       887
      DO 718 II=1,NUINJ                                                      AL       888
      I=IUINJ(II)-1                                                          AL       889
      J=JUINJ(II)                                                            AL       890
      M1=J-1                                                                 AL       891
      IF (J.EQ.JWLI(I,NGOTO)+1) M1=J+1                                       AL       892
      M2=AMAX0(J,M1)                                                         AL       893
      SHRSTR=CFR*.5*(RHO(I,M1,K)+RHO(I,M1,K-1))*W(I,M1,K)                    AL       894
      SHRSTR=ABS(SHRSTR)                                                     AL       895
      SP(I,M1)=SP(I,M1)-SHRSTR*RM(M2)*ZSW(K)*XS(I)                           AL       896
      SHRSTR=CFR*.5*(RHO(I-1,J,K)+RHO(I-1,J,K-1))*W(I-1,J,K)                 AL       897
      SHRSTR=ABS(SHRSTR)                                                     AL       898
      SP(I-1,J)=SP(I-1,J)-SHRSTR*YSR(J)*ZSW(K)                               AL       899
      SU(I,J)=1.E30*WUINJ(II)                                                AL       900
  718 SP(I,J)=-1.E30                                                         AL       901
502   CONTINUE                                                               AL       902
COME HERE FOR DROPLET EVAPORATION TERMS                                      AL       903
      IF (NFNZ.LE.0) GO TO 325                                               AL       904
      READ (NTP4) EVSU                                                       AL       905
      DO 326 J=2,M                                                           AL       906
      KJK=(K-2)*(NI-2)*(NJ-2)+(J-2)*(NI-2)                                   AL       907
      IS=IWLI(J,NGOTO)                                                       AL       908
      IE=IWLO(J,NGOTO)                                                       AL       909
      DO 326 I=IS,IE                                                         AL       910
      LPC=KJK+(I-1)                                                          AL       911
      LZMC=LPC-(NI-2)*(NJ-2)                                                 AL       912
      LIJ=(J-2)*(NI-2)+(I-1)                                                 AL       913
      SU(I,J)=SU(I,J)+EVSU(LIJ)                                              AL       914
      SP(I,J)=SP(I,J)-FZM(K-1)*EVAP(LZMC)                                    AL       915
      IF (K.EQ.NP1) GO TO 347                                                AL       916
      SP(I,J)=SP(I,J)-FZP(K)*EVAP(LPC)                                       AL       917
      GO TO 326                                                              AL       918
  347 SP(I,J)=SP(I,J)-FZP(2)*EVAP(LIJ)                                       AL       919
  326 CONTINUE                                                               AL       920
  325 CONTINUE                                                               AL       921
C +-+-+-+-+-+-+-+-+-+    TURBULENT KINETIC ENERGY    +-+-+-+-+-+-+-+-+-+-+ AL       922
  500 IF (NV.NE.LVK) GO TO 600                                               AL       923
COME HERE FOR SLOT MODIFICATIONS                                             AL       924
      IF (NUINJ.LE.0) GO TO 602                                              AL       925
      DO 731 II=1,NUINJ                                                      AL       926
      I=IUINJ(II)-1                                                          AL       927
      J=JUINJ(II)                                                            AL       928
      M1=J-1                                                                 AL       929
      IF (J.EQ.JWLI(I,NGOTO)+1) M1=J+1                                       AL       930
      WALKE=CFR*.25*((U(I,M1,K)+U(I+1,M1,K))**2+(W(I,M1,K)+W(I,M1,K+1))      AL       931
     1  **2)/RTCO                                                            AL       932
      WALKE=AMAX1(WALKE,1.)                                                  AL       933
      SKE=AKEAC*(UINJ(II)**2+WUINJ(II)**2)                                   AL       934
      SU(I,J)=1.E30*SKE                                                      AL       935
      SP(I,J)=-1.E30                                                         AL       936
      SU(I,M1)=1.E30*WALKE                                                   AL       937
  731 SP(I,M1)=-1.E30                                                        AL       938
```

```
  602 CONTINUE                                                          AL       939
C +-+-+-+-+-+-+-+-+-+-+-+-+-+-   V-VELOCITY   +-+-+-+-+-+-+-+-+-+-+-+-+-+- AL       940
600   IF(NV.NE.2) GO TO 700                                             AL       941
COME HERE FOR SLOT MODIFICATIONS                                        AL       942
      IF (NUINJ.LE.0) GO TO 733                                         AL       943
      DO 730 II=1,NUINJ                                                 AL       944
      I=IUINJ(II)-1                                                     AL       945
      J=JUINJ(II)                                                       AL       946
      SP(I,J+1)=-1.E30                                                  AL       947
  730 SP(I,J)=-1.E30                                                    AL       948
  733 CONTINUE                                                          AL       949
COME HERE FOR DROPLET EVAPORATION TERMS                                 AL       950
      IF (NFNZ.LE.0) GO TO 323                                          AL       951
      READ (NTP4) EVSU                                                  AL       952
      DO 324 J=3,M                                                      AL       953
      KJK=(K-2)*(NI-2)*(NJ-2)+(J-2)*(NI-2)                              AL       954
      IS=IWLI(J,NGOTO)                                                  AL       955
      IE=IWLO(J,NGOTO)                                                  AL       956
      DO 324 I=IS,IE                                                    AL       957
      LPC=KJK+(I-1)                                                     AL       958
      LYNC=LPC-(NI-2)                                                   AL       959
      LIJ=(J-2)*(NI-2)+(I-1)                                            AL       960
      SU(I,J)=SU(I,J)+FVSU(LIJ)                                         AL       961
      SP(I,J)=SP(I,J)-FYM(J-1)*EVAP(LYNC)-FYP(J)*EVAP(LPC)              AL       962
      IF (J.EQ.3) SP(I,J)=SP(I,J)-FYP(2)*EVAP(LYNC)                     AL       963
      IF (J.EQ.M) SP(I,J)=SP(I,J)-FYM(M)*EVAP(LPC)                      AL       964
  324 CONTINUE                                                          AL       965
  323 CONTINUE                                                          AL       966
C +-+-+-+-+-+-+-+-+-+-+-+-+-+-   ENTHALPY   +-+-+-+-+-+-+-+-+-+-+-+-+-+- AL       967
  700 IF (NV.NE.LVH) GO TO 800                                          AL       968
COME HERE FOR CYLINDRICAL WALL SOURCE TERMS                             AL       969
      DO 801 I=2,L                                                      AL       970
      J=JWLO(I,NGOTO)-1                                                 AL       971
      IF (IKIN(I,K).EQ.2.OR.IKIN(I,K).EQ.3) GO TO 1801                  AL       972
      HTC=.5*SQRT((U(I,J,K)+U(I+1,J,K))**2+(W(I,J,K)+W(I,J,K+1))**2)    AL       973
     1  *RHO(I,J,K)*CFR                                                 AL       974
      SU(I,J)=SU(I,J)+HTC*RM(J+1)*ZS(K)*XS(I)*CP*(TCYLW-TEMP(I,J,K))    AL       975
      IF (IDW) 801,801,1801                                             AL       976
 1801 J=JWLI(I,NGOTO)+1                                                 AL       977
      IF (IKIN(I,K).EQ.1.OR.IKIN(I,K).EQ.3) GO TO 801                   AL       978
      HTC=.5*SQRT((U(I,J,K)+U(I+1,J,K))**2+(W(I,J,K)+W(I,J,K+1))**2)    AL       979
     1  *RHO(I,J,K)*CFR                                                 AL       980
      SU(I,J)=SU(I,J)+HTC*RM(J)*ZS(K)*XS(I)*CP*(TCYLW-TEMP(I,J,K))      AL       981
801   CONTINUE                                                          AL       982
COME HERE FOR SLOT MODIFICATIONS                                        AL       983
      IF (NUINJ.LE.0) GO TO 802                                         AL       984
      DO 736 II=1,NUINJ                                                 AL       985
      I=IUINJ(II)-1                                                     AL       986
      J=JUINJ(II)                                                       AL       987
      M1=J-1                                                            AL       988
      IF (J.EQ.JWLI(I,NGOTO)+1) M1=J+1                                  AL       989
      M2=AMAX0(J,M1)                                                    AL       990
      HTC=.5*(W(I-1,J,K)+W(I-1,J,K+1))*RHO(I-1,J,K)*CFR                 AL       991
      HTC=AMAX1(ABS(HTC),1.E-20)                                        AL       992
      SU(I-1,J)=SU(I-1,J)+HTC*YSR(J)*ZS(K)*CP*(TLIP-TEMP(I-1,J,K))      AL       993
      HTC=.5*SQRT((U(I,M1,K)+U(I+1,M1,K))**2+(W(I,M1,K)+W(I,M1,K+1))    AL       994
     1  **2)*RHO(I,M1,K)*CFR                                            AL       995
      SU(I,M1)=SU(I,M1)+HTC*RM(M2)*ZS(K)*XS(I)*CP*(TLIP-TEMP(I,M1,K))   AL       996
      IHCPS=3                                                           NOX      109
      NS1=IDO2                                                          NOX      110
      NS2=IDN2                                                          NOX      111
      TK=TUINJ(II)                                                      NOX      112
      TKINV=1.000/TK                                                    NOX      113
      SP(IDO2)=RATIO2/SMW(IDO2)                                         NOX      114
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      S2(IDN2)=(1.0-RATIO2)/SMW(IDN2)                                    NOX      115
      CALL HCPS                                                          NOX      116
      HPI=HSUM*UNICON*TK                                                 NOX      117
      SU(I,J)=1.E30*HPI                                                  AL       998
  736 SP(I,J)=-1.E30                                                     AL       999
  802 CONTINUE                                                           AL      1000
COME HERE FOR INLET WALL SOURCE TERMS                                    AL      1001
      DO 803 J=2,M                                                       AL      1002
      I=IWLI(J,NGOTO)                                                    AL      1003
      IF (JKIN(J,K).EQ.1) GO TO 1803                                     AL      1004
      HTC=.5*(W(I,J,K)+W(I,J,K+1))*RHO(I,J,K)*CFR                        AL      1005
      HTC=ABS(HTC)                                                       AL      1006
      AREA=YSR(J)*ZS(K)                                                  AL      1007
      SU(I,J)=SU(I,J)+HTC*AREA*CP*(TINLW-TEMP(I,J,K))                    AL      1008
 1803 I=IWLO(J,NGOTO)                                                    AL      1009
      IF (J.GT.JWOI.AND.J.LT.JWOO) GO TO 803                             AL      1010
      LP=I+JP(J)+KP(K)                                                   AL      1011
      HTC=.5*(W(I,J,K)+W(I,J,K+1))*RHO(I,J,K)*CFR                        AL      1012
      HTC=ABS(HTC)                                                       AL      1013
      AREA=YSR(J)*ZS(K)                                                  AL      1014
      SU(I,J)=SU(I,J)+HTC*AREA*CP*(TINLW-TEMP(I,J,K))                    AL      1015
803   CONTINUE                                                           AL      1016
COME HERE FOR DROPLET EVAPORATION TERMS                                  AL      1017
      IF (NFNZ.LE.0) GO TO 315                                           AL      1018
      DO 316 J=2,M                                                       AL      1019
      KJK=(K-2)*(NI-2)*(NJ-2)+(J-2)*(NI-2)                               AL      1020
      IS=IWLI(J,NGOTO)                                                   AL      1021
      IE=IWLO(J,NGOTO)                                                   AL      1022
      DO 316 I=IS,IE                                                     AL      1023
      LPC=KJK+(I-1)                                                      AL      1024
      IHCPS=3                                                            NOX      118
      NS1=IDFU                                                           NOX      119
      NS2=IDFU                                                           NOX      120
      TK=TFUEL                                                           NOX      121
      TKINV=1.000/TK                                                     NOX      122
      S2(IDFU)=1.000/SMW(IDFU)                                           NOX      123
      HDRFU=HSUM*UNICON*TK                                               NOX      124
      SU(I,J)=SU(I,J)+EVAP(LPC)*HDRFU                                    NOX      125
  316 SP(I,J)=SP(I,J)-EVAP(LPC)                                          AL      1026
  315 CONTINUE                                                           AL      1027
C     +-+-+-+-+-+-+-+-+-+-+  PHI (TOTAL FUEL)  +-+-+-+-+-+-+-+-+-+-+-+-+-+  AL      1028
  400 IF (NV.NE.LVFUOX) GO TO 650                                        AL      1029
COME HERE FOR SLOT MODIFICATIONS                                         AL      1030
      IF (NUINJ.LE.0) GO TO 651                                          AL      1031
      DO 737 II=1,NUINJ                                                  AL      1032
      I=IUINJ(II)-1                                                      AL      1033
      J=JUINJ(II)                                                        AL      1034
      SU(I,J)=0.                                                         AL      1035
  737 SP(I,J)=-1.E30                                                     AL      1036
  651 CONTINUE                                                           AL      1037
COME HERE FOR DROPLET EVAPORATION TERMS                                  AL      1038
      IF (NFNZ.LE.0) GO TO 317                                           AL      1039
      DO 318 J=2,M                                                       AL      1040
      KJK=(K-2)*(NI-2)*(NJ-2)+(J-2)*(NI-2)                               AL      1041
      IS=IWLI(J,NGOTO)                                                   AL      1042
      IE=IWLO(J,NGOTO)                                                   AL      1043
      DO 318 I=IS,IE                                                     AL      1044
      LPC=KJK+(I-1)                                                      AL      1045
      SU(I,J)=SU(I,J)+EVAP(LPC)                                          AL      1046
  318 SP(I,J)=SP(I,J)-EVAP(LPC)                                          AL      1047
  317 CONTINUE                                                           AL      1048
C +-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+  FUEL  +-+-+-+-+-+-+-+-+-+-+-+-+-+  AL      1049
  950 IF (NV.NE.LVFU) GO TO 941                                          AL      1050
COME HERE FOR SLOT MODIFICATIONS                                         AL      1051
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      IF (NUINJ.LE.0) GO TO 899                                          AL      1052
      DO 742 II=1,NUINJ                                                  AL      1053
      I=IUINJ(II)-1                                                      AL      1054
      J=JUINJ(II)                                                        AL      1055
  742 SP(I,J)=-1.E30                                                     AL      1056
  899 CONTINUE                                                           AL      1057
COME HERE FOR DROPLET EVAPORATION TERMS                                  AL      1058
      IF (NFNZ.LE.0) GO TO 319                                           AL      1059
      DO 320 J=2,M                                                       AL      1060
      KJK=(K-2)*(NI-2)*(NJ-2)+(J-2)*(NI-2)                               AL      1061
      IS=IWLI(J,NGOTO)                                                   AL      1062
      IE=IWLO(J,NGOTO)                                                   AL      1063
      DO 320 I=IS,IE                                                     AL      1064
      LPC=KJK+(I-1)                                                      AL      1065
      SU(I,J)=SU(I,J)+EVAP(LPC)                                          AL      1066
  320 SP(I,J)=SP(I,J)-EVAP(LPC)                                          AL      1067
  319 CONTINUE                                                           AL      1068
C     +-+-+-+-+-+-+-+-+-+-+-+-+-      CO          +-+-+-+-+-+-+-+-+-+-+-+-+- AL      1069
  941 IF(NV.NE.LVCO.AND.NV.NE.LVCH.AND.NV.NE.LVH2.AND.NV.NE.LVH1)GO TO   4STEP   173
     1 950                                                               4STEP   174
COME HERE FOR SLOT MODIFICATION                                          AL      1071
      IF(NUINJ.LE.0) GO TO 959                                           AL      1072
      DO 952 II=1,NUINJ                                                  AL      1073
      I=IUINJ(II)-1                                                      AL      1074
      J=JUINJ(II)                                                        AL      1075
      SU(I,J)=0.                                                         AL      1076
  952 SP(I,J)=-1.E30                                                     AL      1077
  959 CONTINUE                                                           AL      1078
COME HERE FOR DROPLET EVAPORATION TERMS                                  AL      1079
  951 IF (NFNZ.LE.0) GO TO 950                                           AL      1080
      DO 957 J=2,M                                                       AL      1081
      KJK=(K-2)*(NI-2)*(NJ-2)+(J-2)*(NI-2)                               AL      1082
      IS=IWLI(J,NGOTO)                                                   AL      1083
      IE=IWLO(J,NGOTO)                                                   AL      1084
      DO 957 I=IS,IE                                                     AL      1085
      LPC=KJK+(I-1)                                                      AL      1086
  957 SP(I,J)=SP(I,J)-EVAP(LPC)                                          AL      1087
C+-+-+-+-+-+-+-+-+-+-+-+-+-  NUCLEI CONCENTRATION  +-+-+-+-+-+-+-+-+-+-+-+-+ SOOT    118
  950 IF(NV.NE.LVN)GO TO 1200                                            SOOT    119
COME HERE FOR SLOT MODIFICATIONS                                         SOOT    120
      IF(NUINJ.LE.0)GO TO 1203                                           SOOT    121
      DO 1207 II=1,NUINJ                                                 SOOT    122
      I=IUINJ(II)-1                                                      SOOT    123
      J=JUINJ(II)                                                        SOOT    124
      SU(I,J)=0.0                                                        SOOT    125
 1207 SP(I,J)=-1.0E30                                                    SOOT    126
COME HERE FOR DROPLET EVAPORATION TERMS                                  SOOT    127
 1203 IF(NFNZ.LE.0)GO TO 1205                                            SOOT    128
      DO 1206 J=2,M                                                      SOOT    129
      KJK=(K-2)*(NI-2)*(NJ-2)+(J-2)*(NI-2)                               SOOT    130
      IS=IWLI(J,NGOTO)                                                   SOOT    131
      IE=IWLO(J,NGOTO)                                                   SOOT    132
      DO 1206 I=IS,IE                                                    SOOT    133
      LPC=KJK+I-1                                                        SOOT    134
 1206 SP(I,J)=SP(I,J)-EVAP(LPC)                                          SOOT    135
 1205 CONTINUE                                                           SOOT    136
      RETURN                                                             SOOT    137
C+-+-+-+-+-+-+-+-+-+-  SOOT CONCENTRATION  +-+-+-+-+-+-+-+-+-+-+-+-+-+-+ SOOT    138
 1200 IF(NV.LT.LVS1.OR.NV.GT.LVS2)GO TO 1300                             SOOT    139
COME HERE FOR SLOT MODIFICATIONS                                         SOOT    140
      IF(NUINJ.LE.0)GO TO 1303                                           SOOT    141
      DO 1302 II=1,NUINJ                                                 SOOT    142
      I=IUINJ(II)-1                                                      SOOT    143
      J=JUINJ(II)                                                        SOOT    144
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      SU(I,J)=0.0                                                       SOOT     145
 1304 SP(I,J)=-1.0E30                                                   SOOT     146
CONE HERE FOR DROPLET EVAPORATION TERMS                                 SOOT     147
 1303 IF(NFNZ.LE.0)GO TO 1305                                           SOOT     148
      DO 1306 J=2,M                                                     SOOT     149
      KJK=(K-2)*(NI-2)*(NJ-2)+(J-2)*(NI-2)                              SOOT     150
      IS=IWLI(J,NGOTO)                                                  SOOT     151
      IE=IWLO(J,NGOTO)                                                  SOOT     152
      DO 1306 I=IS,IE                                                   SOOT     153
      LPC=KJK+I-1                                                       SOOT     154
 1306 SP(I,J)=SP(I,J)-EVAP(LPC)                                         SOOT     155
 1305 CONTINUE                                                          SOOT     156
      RETURN                                                            SOOT     157
C +-+-+-+-+-+-+-+-+-+-+-+   X-DIRECTION RADIATION   +-+-+-+-+-+-+-+-+-+-+-+-+  AL      1089
 1300 IF(NV.NE.LVRX)GO TO 910                                           SOOT     158
C-----INLET BOUNDARY.                                                   COMMENT   60
      DO 901 J=2,M                                                      AL      1091
      I=IWLI(J,NGOTO)                                                   AL      1092
      IF (JKIN(J,K).EQ.1) GO TO 902                                     AL      1093
      TEMPW=TEMP(I-1,J,K)                                               AL      1094
      SU(I,J)=SU(I,J)+EMI*SIGMA*TEMPW**4                                AL      1095
      SP(I,J)=SP(I,J)-EMI                                               AL      1096
      GO TO 1901                                                        AL      1097
902   CONTINUE                                                          AL      1098
      SU(I,J)=SU(I,J)+RADIN                                             AL      1099
      SP(I,J)=SP(I,J)-1.                                                AL      1100
C-----OUTLET BOUNDARY.                                                  COMMENT   61
 1901 I=IWLO(J,NGOTO)                                                   AL      1101
      IF (J.GT.JWOI.AND.J.LT.JWOO) GO TO 1902                           AL      1102
      TEMPW=TEMP(I+1,J,K)                                               AL      1103
      SU(I,J)=SU(I,J)+EMI*SIGMA*TEMPW**4                                AL      1104
      SP(I,J)=SP(I,J)-EMI                                               AL      1105
      GO TO 901                                                         AL      1106
 1902 CONTINUE                                                          AL      1107
      SU(L,J)=SU(L,J)+RADSUR                                            AL      1108
      SP(L,J)=SP(L,J)-1.                                                AL      1109
901   CONTINUE                                                          AL      1110
CONE HERE FOR SLOT MODIFICATIONS                                        AL      1111
      IF (NUINJ.LE.0) GO TO 903                                         AL      1112
      DO 743 II=1,NUINJ                                                 AL      1113
      I=IUINJ(II)-1                                                     AL      1114
      J=JUINJ(II)                                                       AL      1115
      SU(I+1,J)=SU(I+1,J)+EMISR*SIGMA*TEMP(I,J,K)**4                    AL      1116
      SP(I+1,J)=SP(I+1,J)-1                                             AL      1117
      TEMPW=TLIP                                                        AL      1118
      SU(I-1,J)=SU(I-1,J)+EMI*SIGMA*TEMPW**4                            AL      1119
  743 SP(I-1,J)=SP(I-1,J)-EMI                                           AL      1120
 903  CONTINUE                                                          AL      1121
C +-+-+-+-+-+-+-+-+-+-+-+   Y-DIRECTION RADIATION   +-+-+-+-+-+-+-+-+-+-+-+-+  AL      1122
  910 IF (NV.NE.LVRY) GO TO 920                                         AL      1123
      DO 911 I=2,L                                                      AL      1124
C-----TOP WALL.                                                         COMMENT   62
      J=JWLO(I,NGOTO)-1                                                 AL      1125
      IF (IKIN(I,K).EQ.2.OR.IKIN(I,K).EQ.3) GO TO 904                   AL      1126
      TEMPW=TEMP(I,J+1,K)                                               AL      1127
      SU(I,J)=SU(I,J)+EMI*SIGMA*TEMPW**4*RM(J+1)                        AL      1128
      SP(I,J)=SP(I,J)-EMI*RM(J+1)                                       AL      1129
      GO TO 905                                                         AL      1130
  904 SU(I,J)=SU(I,J)+RADIN*RM(J+1)                                     NASAX     24
      SP(I,J)=SP(I,J)-RM(J+1)                                           NASAX     25
  905 IF (IOW) 911,911,1911                                             AL      1133
C-----BOTTOM WALL.                                                      COMMENT   63
 1911 J=JWLI(I,NGOTO)+1                                                 AL      1134
      IF (IKIN(I,K).EQ.1.OR.IKIN(I,K).EQ.3) GO TO 906                   AL      1135
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      TEMPW=TEMP(I,J-1,K)                                                AL      1136
      SU(I,J)=SU(I,J)+EMI*SIGMA*TEMPW***4*RM(J)                          AL      1137
      SP(I,J)=SP(I,J)-EMI*RM(J)                                          AL      1138
      GO TO 911                                                          AL      1139
  906 SU(I,J)=SU(I,J)+RADIN*RM(J)                                        NASAX     26
      SP(I,J)=SP(I,J)-RM(J)                                              NASAX     27
911   CONTINUE                                                           AL      1142
C-----SLOT MODIFICATIONS.                                                COMMENT   64
      IF (NUINJ.LE.0) GO TO 912                                          AL      1143
      DO 744 II=1,NUINJ                                                  AL      1144
      I=IUINJ(II)-1                                                      AL      1145
      J=JUINJ(II)                                                        AL      1146
      M1=J-1                                                             AL      1147
      IF (J.EQ.JWLI(I,NGOTO)+1) M1=J+1                                   AL      1148
      M2=MAX0(J,M1)                                                      AL      1149
      TE  'W=TLIP                                                        AL      1150
      SU.I,M1)=SU(I,M1)+EMI*SIGMA*TEMPW***4*RM(M2)                       AL      1151
  744 SP(I,M1)=SP(I,M1)-EMI*RM(M2)                                       AL      1152
912   CONTINUE                                                           AL      1153
  920 CONTINUE                                                           AL      1154
      RETURN                                                             AL      1155
C **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  AL      1156
C -+-+-+-+-+-+-+-+-+-+-+-+  Z-DIRECTION RADIATION  -+-+-+-+-+-+-+-+-+-+-+ AL      1157
      ENTRY SOMODZ                                                       AL      1158
C-----SLOT MODIFICATIONS.                                                COMMENT   65
      IF (NUINJ.LE.0) GO TO 1100                                         AL      1159
      DO 1102 II=1,NUINJ                                                 AL      1160
      IF (JUINJ(II).NE.JPLANE) GO TO 1102                                AL      1161
      I=IUINJ(II)-1                                                      AL      1162
      DO 1104 K=2,N                                                      AL      1163
      SU(I,K)=0.                                                         AL      1164
 1104 SP(I,K)=-1.E30                                                     AL      1165
 1102 CONTINUE                                                           AL      1166
 1100 CONTINUE                                                           AL      1167
C-----CYCLIC BOUNDARY CONDITIONS.                                        COMMENT   66
      DO 921 I=2,L                                                       AL      1168
      LP2=I+JM(JPLANE)+KN(2)                                             AL      1169
      LPN=I+JM(JPLANE)+KN(N)                                             AL      1170
      GAMDDL=.5*(GAM(I,JPLANE,2)+GAM(I,JPLANE,N))/R(JPLANE)/(ZDIF(NP1)+  AL      1171
     1       ZDIF(2))                                                    AL      1172
      SU(I,2)=SU(I,2)+GAMDDL*F(LPN,NVRZ)                                 AL      1173
      SP(I,2)=SP(I,2)-GAMDDL                                             AL      1174
      SU(I,N)=SU(I,N)+GAMDDL*F(LP2,NVRZ)                                 AL      1175
      SP(I,N)=SP(I,N)-GAMDDL                                             AL      1176
921   CONTINUE                                                           AL      1177
      RETURN                                                             AL      1178
      END                                                                AL      1179
      SUBROUTINE OUTPUT(NTP)                                             OU         2
      COMMON F(500,7),DU(10,10,5),DV(10,10,5),DW(10,10,5),               COMFA      2
     1 ANUC(10,10,5),SOOT1(10,10,5),SOOT2(10,10,5),FCN(10,10,5),         4STEP      1
     2 EM2(10,10,5),ES(500,14),                                          4STEP      2
     1 RHO(10,10,5),VISC(10,10,5),ABSR(10,10,5),SCTR(10,10,5),           RAD        1
     1 SU(10,10),SP(10,10),DRHODP(10,10,5),                              RAD        2
     1  AXP(10,10),AXM(10,10),AYP(10,10),AYM(10,10),AZP(10,10),          COMFA      4
     2  AZM(10,10),C7(10,10),CY(10),CZU(10,10),CYU(10),                  COMFA      5
     3  C7P(10,10),CYP(10),DIVG(10,10),NTP1,NTP2                         COMFA      6
     1,AXMK(192),AXPK(192),AYMK(192),AYPK(192),AZMK(192),AZPK(192),      CTOMA      1
     2 SUK(192),SPK(192)                                                 CTOMA      2
      DIMENSION U(10,10,5),V(10,10,5),W(10,10,5),PP(10,10,5)             COMFA      7
      DIMENSION P(10,10,5),TEMP(10,10,5),GAM(10,10,5)                    COMFA      8
      EQUIVALENCE (F(1,1),U(1,1,1)),(F(1,2),V(1,1,1)),(F(1,3),W(1,1,1))  COMFA      9
      EQUIVALENCE (F(1,4),PP(1,1,1)),(F(1,5),P(1,1,1))                   COMFA     10
      EQUIVALENCE (F(1,6),TEMP(1,1,1)),(F(1,7),GAM(1,1,1))               COMFA     11
      COMMON/CYL/R(30),RM(30),RMV(30),YSR(30),YSVR(30),JPLAX             COMMON     2
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      COMMON/GRID/X(40),Y(30),Z(30),XS(40),YS(30),ZS(30),XSU(40),      COMMON    3
     1   YSV(30),ZSW(30),XDIF(40),YDIF(30),ZDIF(30),FXP(40),FXM(40),    COMMON    4
     2   FYP(30),FYM(30),FZP(30),FZM(30),DT,TIME                        COMMON    5
      COMMON
     1/CINDEX/IDCO,IDFU,IDO2,IDN2,IDH2O,IDCO2,IDH1,IDH2,IDN1,IDNO,IDNO2 NOX       2
     1,IDO,IDOH,IHCPS,ILC,ILH,IMAT,ITER,JJJ,M1,M2,M3,MA,NGLOB,NGLOBP,   NOX       3
     2 NLM,NQ,NSM,NS1,NS2,IDCH                                          NOX       4
     3/CCHEM1/CPSUP,HSUM,FQ,PPLN,RGAS,RGASIN,SMINV,TKINV,TLN,LNRG       4STEP     3
     4/CPARAM/ASUB(30,3),EMV,ER,HSURO,NDEBUG,NS,PA,QQ,Q1,Q2,Q3,Q4,RHOPP, NOX       6
     4 SM,SMW(30),SMQ,S1(30),S2(30),TK,LADIAB,LDEBUG,LEQUIL,LREACT,     NOX       7
     4 LENER,FDKIJ,LCONVG                                               NOX       8
      DOUBLE PRECISION CPSUM,EMV,ER,FQ,HSURO,HSUM,PA,PPLN,QQ,Q1,Q2,Q3,  NOX       9
     1 Q4,RGAS,RGASIN,RHOPP,SM,SMINV,SMW,S1,S2,TK,TKINV,TLN,SMQ         NOX      10
     2,FUT,FST                                                          NOX      11
      COMMON/STEP4/PEXP1,PEXP2,PEXP3,PEXP4,ER1,ER2,ER3,ER4,CEBU1,CEBU2, 4STEP     4
     1 CEBU3,CEBU4,AEXP1,AEXP2,AEXP3,AEXP4,BEXP1,BEXP2,BEXP3,BEXP4,     4STEP     5
     2 CEXP1,CEXP2,CEXP3,CEXP4,FUT,FST                                  4STEP     6
      LOGICAL LADIAB,LCONVG,LDEBUG,LEQUIL,LNRG,LREACT,LENER             4STEP     7
      COMMON/INT/L,M,N,LCV,MCV,NCV,LP1,MP1,NP1,NI,NJ,NK,NIMJ,NIMJNK,NV,  NOX      12
     1 NMV,NGOTO,K,ISTR,JSTR,KSTR,NVM(35),KM(30),JM(30),ISTEP,          COMMON    6
     2 ISOLVE(32),IPRINT(33),TITLE(10,33),IXY,ISWP,JSWP,RELAX(35),NP,   4STEP     8
     3  NRHO,NGAM,IWLI(30,5),IWLO(30,5),JWLO(40,5),JWLI(40,5),IWEI,     4STEP     9
     4  IWFO,MM1,JWII,JWIO,JWOI,JWOO,IDW,JKIN(30,30),IKIN(40,30)        COMMON    9
      COMMON/INDEX/IPAR,LPREF,ISTUN,INCOMP,ITRAD,NVRX,NVRY,NVRZ,JPLANE  COMMON   10
     1,PLANM1,LVA,LVD,LVFUOX,LVFU,LVCO,LVH,LVRX,LVRY,LVRZ,NVF(32),      COMMON   11
     2  IJUMP,IRES,TITLE2(20),IMAX,JMAX,KMAX,NVCO,FUNCO,NVH2O,NVCO2,    4STEP    10
     3 NVN2,NVCH,NVH2                                                   COMMON   13
      COMMON/CNOX/LVH1,LVH2,LVN1,LVNO,LVNO2,LVO,LVOH,LVH2O,LVN2,LVO2,   4STEP    11
     1 LVCO2,LVFU1,LVCO1,NNOX,INOX,ITNOX,SNOX,TNOX                      NOX      16
      COMMON/THERM/NVH,NVFU,NVOX,NVFUOX,NVTE,NODEN,IDK,FSTOIC,HFU,CP,   NOX      17
     1  GASCON,RHOCON,UNICON,PRESS,NVFAV,TCYLW,TINLW,TLIP,ACOEF(4),     COMMON   15
     2  T4,OFAC,WFU,WCO2,WCO,WOX,WH2O,WN2,HYY,CXX,RATIO1,RATIO2,        COMMON   16
     3  RATIO3,RATIO4,HCO,TAN,ITHALL                                    COMMON   17
      COMMON/CTCMA/NEND,ICTOMA(32)                                      COMMON   18
      COMMON/MISCAMU/DEN,SMAX,SSUM,LASTEP,HTCEXT,CFR,EMISW,EMISIN,      4STEP    12
     1  EMISR,TOUT,RTCO,EMI,RADIN,RADSUR,FNA,FK,SOFK,                   CONGEN    2
     2  FXFU,FOFU,TFUEL,NFNZ,FLO(40),TENTH(40),H(40),FUEL(40),FUOX(40),  CONGEN    3
     2 UIN(40),TIN(40),FUELS(40),SEXIT,IGAN1(29),IGAN2(29)              CONGEN    4
      COMMON/TURB/NNK,NVD,C1,C2,CD,AK,DUIDXJ(3,3),AKFAC,ALFAC,          4STEP    13
     1 MODEL,PR(32),PREF(32),PJAY(32),E                                 CONGEN    6
      COMMON/RAD/NVE,SIGMA,ABSOR,SCATR                                  4STEP    14
      COMMON/REACT/ARCON1,PREXP1,CR1,ARCON2,PREXP2,CR2,MODER            CONGEN    8
      COMMON/DROPL/EVAP(192),NTP4,NFNZ,XO(3),YO(3),ZO(3),ALFA(3),       CONGEN    9
     1  BETA(3),DELTA(3),THETA1(3),THETA2(3),NSL(3),WFF(3),SMD(3),      CONGEN   10
     2  VFUEL(3),RFUEL(3),EVSU(64),NEVAP                                CONGEN   11
      COMMON/INJEC/FLOWIN,XUINJ(20),JUINJ(20),UINJ(20),WUINJ(20),       CONGEN   12
     1  AUINJ(20),TUINJ(20),IVINJ(20),JVINJ(20),KVINJ(20),VINJ(20),     CONGEN   13
     2  EVINJ(20),DVINJ(20),AVINJ(20),TVINJ(20),NUINJ,NVINJ,JSW1,JSW2,  CONGEN   14
     3  USW,VSW,AFSW,FSW,TSW,WSW,SWNO,RHOSW                             CONGEN   15
      COMMON/CSOOT/NVN,NVS1,NVS2,ISOOT,SSOOT,NSOOT,AO,ARCONN,AAA,ABB,FNG SOOT     8
     1,GO,MPART,DPART(2),FRACP(2),RHOP,ARCONS,PREXPS,ALPHA,AAS,ABS,DHR   SOOT     9
      COMMON/CRAD/IRAD,SRAD                                             SOOT    10
      COMMON/CFOUR/PREXP3,ARCON3,CR3,PREXP4,ARCON4,CR4,AA1,BB1,CC1,     SOOT    11
     1 AA2,BB2,CC2,AA3,BB3,CC3,AA4,BB4,CC4,RATIO5,RATIO6,RATIO7,        4STEP    15
     2 RATIO8,RATIO9,RATO10,RATO11,RATO12,WCH,WH2,WC2H4,LVCH,LVCH1,LVH21 4STEP    16
C------SUBROUTINE OUTPUT IS USED FOR PRINTOUT PURPOSES.                 4STEP    17
C                                                                       COMMENT  67
      IF (NTP.LE.0) GO TO 16                                            COMMENT  68
      IF (ISTEP.EQ.LASTEP) GO TO 11                                     OU        6
      IF (MOD(ISTEP,IJUMP)) 20,11,20                                    OU        7
   11 CONTINUE                                                          OU        8
      REWIND NTP                                                        OU        9
      READ (NTP) U,V,W,P                                                OU       10
                                                                        OU       11
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      CALL FPRINT (1,3,1)                                                OU        12
      CALL FPRINT (5,5,4)                                                OU        13
      IF(ISTEP.EQ.0)GO TO 300                                            NOX      127
      IF(MSOOT.EQ.0)GO TO 227                                            SOOT     159
C-----SOOT EMISSIONS INDEX AND SMOKE NUMBER.                             COMMENT   69
      FLOW=0.0                                                           SOOT     160
      PBAR=0.0                                                           SOOT     161
      SBAR=0.0                                                           SOOT     162
      DO 225 K=2,N                                                       SOOT     163
      DO 225 J=2,M                                                       SOOT     164
      LP=KM(K)+JM(J)+L                                                   SOOT     165
      DMOOT=RHO(LP1,J,K)*YSR(J)*ZS(K)*U(LP1,J,K)                         SOOT     166
      FLOW=FLOW+DMOOT                                                    SOOT     167
      DSOOT=DMOOT*(SOOT1(L,J,K)+SOOT2(L,J,K))                            SOOT     168
      SBAR=SBAR+DSOOT                                                    SOOT     169
  225 PBAR=PBAR+DSOOT*RHO(LP1,J,K)                                       SOOT     170
      PBAR=PBAR*1.0E-30                                                  SOOT     171
      FLOW=FLOW*1.0E-30                                                  SOOT     172
      CSMO=1000.0*SBAR/FUTOT                                             SOOT     173
      SMCONC=1.0E6*PBAR/FLOW                                             SOOT     174
      SMONO=12.5847*ALOG(SMCONC)+12.045                                  SOOT     175
      SMONO=AMAX1(SMONO,0.0)                                             SOOT     176
  227 IF(MNOX.EQ.0)GO TO 300                                             NOX      128
C-----NOX EMISSIONS INDEX.                                               COMMENT   70
      PBAR=0.0                                                           NOX      129
      DO 301 K=2,N                                                       NOX      130
      DO 301 J=2,M                                                       NOX      131
      LP=KM(K)+JM(J)+L                                                   NOX      132
  301 PBAR=PBAR+RHO(LP1,J,K)*YSR(J)*ZS(K)*U(LP1,J,K)*(F(LP,LVNO)*46./30.  NOX      133
     1+F(LP,LVNO2))                                                      NOX      134
      CNO=1000.0*PBAR/FUTOT                                              NOX      135
  300 CONTINUE                                                           NOX      136
C  ----   HERE PP IS ACTUALLY KE,  P IS ACTUALLY DISSIPATION             OU        14
      READ (NTP) PP,P                                                    OU        15
      DO 25 K=1,NP1                                                      OU        16
      DO 25 J=1,MP1                                                      OU        17
      KJM=KM(K)+JM(J)                                                    OU        18
      DO 25 I=1,LP1                                                      OU        19
      LP=KJM+I                                                           OU        20
   25 F(LP,NVD)=CD*F(LP,NVK)**1.5/(F(LP,NVD)+1.0E-30)                    OU        21
      CALL FPRINT (NVK,NVD,5)                                            OU        22
C -------- HERE PP IS PHI, P IS MFU, OU IS MCO                           OU        23
      READ (NTP) PP,P,OU                                                 OU        24
      CALL FPRINT (NVFUOX,NVTE,7)                                        OU        25
      CALL FPRINT (NVCO,NVCO,15)                                         OU        26
      DO 50 K=1,NP1                                                      OU        27
      DO 50 J=1,MP1                                                      OU        28
      KJM=KM(K)+JM(J)                                                    OU        29
      DO 50 I=1,LP1                                                      OU        30
      LP=KJM+I                                                           OU        31
      FUR=F(LP,NVFUOX)-F(LP,NVFU)                                        OU        32
      F(LP,NVCO2)=FS(LP,IOCO2)                                           NOX      137
      F(LP,NVOX)=FS(LP,IOO2)                                             NOX      138
      F(LP,NVH2O)=FS(LP,IOH2O)                                           NOX      139
      F(LP,NVN2)=FS(LP,ION2)                                             NOX      140
   50 CONTINUE                                                           OU        40
      CALL FPRINT (NVH2O,NVN2,16)                                        OU        41
      IF (NFNZ.LE.0) GO TO 35                                            OU        42
      DO 37 K=1,NP1                                                      OU        43
      DO 37 J=1,MP1                                                      OU        44
      KJM=KM(K)+JM(J)                                                    OU        45
      DO 37 I=1,LP1                                                      OU        46
      LP=KJM+I                                                           OU        47
   37 F(LP,NVFUOX)=0.                                                    OU        48
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C-----SPRAY EVAPORATION RATES.                                          COMMENT    71
      DO 39 K=2,N                                                       OU         49
      DO 39 J=2,M                                                       OU         50
      KJM=KM(K)+JM(J)                                                   OU         51
      KJK=(K-2)*(NI-2)*(NJ-2)+(J-2)*(NI-2)                              OU         52
      DO 39 I=2,L                                                       OU         53
      LP=KJM+I                                                          OU         54
      LPC=KJK+(I-1)                                                     OU         55
   39 F(LP,NVFUOX)=EVAP(LPC)                                            OU         56
      CALL FPRINT (NVFUOX,NVFUOX,22)                                    OU         57
   35 CONTINUE                                                          OU         58
C ------- HERE DV IS ENTHALPY, DW IS FAV                                OU         59
      READ (NTP) DV,DW                                                  OU         60
      CALL FPRINT (NVH,NVFAV,10)                                        OU         61
C  -----   HERE U IS FX,  V IS FY,  W IS FZ                             OU         62
      READ (NTP) U,V,W                                                  OU         63
      CALL FPRINT (NVRX,NVRZ,12)                                        OU         64
C ------- RHO AND VISCOSITY                                            OU         65
      CALL FPRINT(30,30,20)                                             4STEP     175
      NV=4                                                              OU         67
      DO 56 K=1,NP1                                                     OU         68
      DO 56 J=1,MP1                                                     OU         69
      KJM=KM(K)+JM(J)                                                   OU         70
      DO 56 I=1,LP1                                                     OU         71
      LP=KJM+I                                                          OU         72
   56 F(LP,7)=0.                                                        OU         73
      CALL GAMMA                                                        OU         74
      CALL FPRINT (7,7,21)                                              OU         75
      REWIND NTP1                                                       OU         76
      DO 46 II=1,2                                                      OU         77
   46 READ (NTP1)                                                       OU         78
C --------- HERE PP IS PHI, P IS MFU, DU IS MCO                         OU         79
      READ (NTP1) PP,P,DU                                               OU         80
      CALL FPRINT(11,13,23)                                             SOOT      179
      CALL FPRINT(24,29,26)                                             4STEP     176
      CALL FPRINT(14,15,32)                                             4STEP     177
      IF(ISTEP.GT.0.AND.NSOOT.NE.0)WRITE(6,226)SMONO,SMCONC,CSNO        SOOT      180
  226 FORMAT(1HO,10(1H*),5X,*SMOKE NUMBER = *,  E10.2,5X,10(1H*)/1HO,   SOOT      181
     1 10(1H*),5X,*SMOKE CONCENTRATION = *,E10.2,1X,*MG/M3, OR*,E10.2,  SOOT      182
     2 1X,*GM.OF SMOKE/KG.OF FUEL*,5X,10(1H*)/)                         SOOT      183
      IF(ISTEP.GT.0.AND.NNOX.NE.0)WRITE(6,302)CNO                       NOX       143
  302 FORMAT(1HO,10(1H*),5X,*NOX EMISSIONS INDEX = *,E10.2,1X,          NOX       144
     1 *GM.OF NO2/KG.OF FUEL*,5X,10(1H*)/)                              NOX       145
   14 CONTINUE                                                          OU         81
      WRITE(6,19)                                                       OU         82
   19 FORMAT (1HO,4HSTEP,5X,4HSMAX,7X,4HSSUM,6X,5HSERIT,5X,             OU         83
     1   8HP(2,M,2),3X,8HP(L,M,2),3X,8HU(I,J,K),3X,8HV(I,J,K),3X,       OU         84
     2   8HW(I,J,K),2X,8HT(I,J,K),2X,10HRHO(I,J,K),2X,7HI   J   K)      OU         85
20    CONTINUE                                                          OU         86
      RETURN                                                            OU         87
      END                                                               OU         88
      SUBROUTINE AUX                                                    AU          2
      COMMON F(35001),DU(500),DV(500),DW(500),                          COMFB      2
     1 ANUC(500),SOOT1(500),SOOT2(500),FCH(500),FH2(500),FS(500,14),    4STEP      10
     1 RHO(500),VISC(500),ABSR(500),SCTR(500),SU(100),SP(100),          RAD        3
     1 DRHODP(500),                                                     RAD        4
     1   AXP(100),AXM(100),AYP(100),AYM(100),AZP(100),                  COMFB      4
     2   AZM(100),CZ(100),CY(10),CZU(100),CYU(10),                      COMFB      5
     3   CZP(100),CYP(10),DIVG(100),NTP1,NTP2                           COMFB      6
     1,AXMK(192),AXPK(192),AYMK(192),AYPK(192),AZMK(192),AZPK(192),     CTOMA      3
     2 SUK(192),SPK(192)                                                CTOMA      4
      DIMENSION U(500),V(500),W(500),PP(500),P(500),TEMP(500)           COMFB      7
      DIMENSION GAM(500)                                                COMFB      8
      EQUIVALENCE (F(1),U(1)),(F(501),V(1)),(F(1001),W(1))              COMFB      9
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      EQUIVALENCE (F(1501),PP(1)),(F(2001),P(1)),(F(2501),TEMP(1))        COMFB    10
      EQUIVALENCE (F(3001),GAM(1))                                        COMFB    11
      COMMON/CYL/R(30),RM(30),RMV(30),YSR(30),YSVR(30),IPLAX              COMMON    2
      COMMON/GRID/X(40),Y(30),Z(30),XS(40),YS(30),ZS(30),XSU(40),         COMMON    3
     1  YSV(30),ZSW(30),XDIF(40),YDIF(30),ZDIF(30),FXP(40),FXM(40),       COMMON    4
     2  FYP(30),FYM(30),FZP(30),FZM(30),DT,TIME                           COMMON    5
      COMMON                                                              NOX       2
     1/CINDEX/IDCO,IDFU,IDO2,IDN2,IDH2O,IDCO2,IDH1,IDH2,IDN1,IDNO,IDNO2   NOX       3
     1,IDO,IDOH,IHCPS,ILC,ILH,IMAT,ITER,JJJ,N1,N2,N3,NA,NGLOB,NGLOBP,     NOX       4
     2 NLM,NO,NSP,NS1,NS2,IOCH                                            4STEP     3
     3/CCHEMI/CPSUM,HSUM,FO,PPLN,RGAS,RGASIN,SMINV,TKINV,TLN,LNRG         NOX       6
     4/CPARAM/ASUB(30,3),ENV,ER,HSUBO,NDEBUG,MS,PA,QO,Q1,Q2,Q3,Q4,RHOPP,  NOX       7
     4 SM,SMW(30),SMO,S1(30),S2(30),TK,LADIAB,LDEBUG,LEQUIL,LREACT,       NOX       8
     4 LENER,FDKIJ,LCONVG                                                 NOX       9
      DOUBLE PRECISION CPSUM,ENV,ER,FO,HSUBO,HSUM,PA,PPLN,QO,Q1,Q2,Q3,    NOX      10
     1 Q4,RGAS,RGASIN,RHOPP,SM,SMINV,SMW,S1,S2,TK,TKINV,TLN,SMO           NOX      11
     2,FUT,FST                                                            4STEP     4
      COMMON/STEP4/PEXP1,PEXP2,PEXP3,PEXP4,ER1,ER2,ER3,ER4,CEBU1,CEBU2,   4STEP     5
     1 CEBU3,CEBU4,AEXP1,AEXP2,AEXP3,AEXP4,BEXP1,BEXP2,BEXP3,BEXP4,       4STEP     6
     2 CEXP1,CEXP2,CEXP3,CEXP4,FUT,FST                                    4STEP     7
      LOGICAL LADIAB,LCONVG,LDEBUG,LEQUIL,LNRG,LREACT,LENER               NOX      12
      COMMON/INT/L,P,N,LCV,NCV,NV,LP1,MP1,NP1,NI,NJ,NK,NINJ,NINJNK,NV,    COMMON    6
     1 NNV,NGOTO,K,ISTR,JSTR,KSTR,NVM(35),KM(30),JM(30),ISTEP,            4STEP     8
     2 ISOLVE(32),IPRINT(33),TITLE(10,33),IXY,ISWP,JSWP,RELAX(35),NP,     4STEP     9
     3  NRHO,NGAM,IWLI(30,5),IWLO(30,5),JWLO(40,5),JWLI(40,5),IWEI,       COMMON    9
     4  IWEO,MM1,JWII,JWIO,JWOI,JWOO,IOW,JKIN(30,30),IKIN(40,30)          COMMON   10
      COMMON/INDEX/IPAR,LPREF,ISTUN,INCOMP,ITRAD,NVRX,NVRY,NVRZ,JPLANE    COMMON   11
     1,PLAXM1,LVK,LVD,LVFUOX,LVFU,LVCO,LVH,LVRX,LVRY,LVRZ,NVF(32),        4STEP    10
     2  IJUMP,IRFS,TITLE2(20),IMAX,JMAX,KMAX,NVCO,FUNCO,NVH2O,NVCO2,      COMMON   13
     3 NVN2,NVCH,NVH2                                                     4STEP    11
      COMMON/CNOX/LVH1,LVH2,LVN1,LVNO,LVNO2,LVO,LVOH,LVH2O,LVN2,LVO2,     NOX      16
     1 LVCO2,LVFU1,LVCO1,NNOX,INOX,ITNOX,SNOX,TNOX                        NOX      17
      COMMON/THERM/NVH,NVFU,NVOX,NVFUOX,NVTE,MODEN,IOK,FSTOIC,HFU,CP,     COMMON   15
     1  GASCON,RHOCON,UNICON,PRESS,NVFAV,TCYLW,TINLW,TLIP,ACOEF(4),       COMMON   16
     2  T4,OFAC,WFU,WCO2,WCO,WOX,WH2O,WN2,HYY,CXX,RATIO1,RATIO2,          COMMON   17
     3  RATIO3,RATIO4,HCO,TAN,ITWALL                                      COMMON   18
      COMMON/CTDMA/KEND,ICTDMA(32)                                        4STEP    12
      COMMON/MIS/APU,DEN,SMAX,SSUM,LASTEP,HTCEXT,CFR,EMISW,EMISIN,        COMGEN    2
     1  EMISR,TOUT,RTCO,EMI,RADIN,RADSUR,FMA,FK,SQFK,                     COMGEN    3
     2  FKFU,FDFU,TFUEL,MFNZ,FLO(40),TEMTM(40),H(40),FUEL(40),FUOX(40) ,   COMGEN    4
     2 UIN(40),TIN(40),FUELS(40),SEXIT,IGAM1(29),IGAM2(29)                4STEP    13
      COMMON/TURB/NVK,NVD,C1,C2,CD,AK,DUIDXJ(3,3),AKFAC,ALFAC,            COMGEN    6
     1 MODEL,PR(32),PREF(32),PJAY(32),E                                   4STEP    14
      COMMON/RAD/NVE,SIGMA,ABSOR,SCATR                                    COMGEN    8
      COMMON/REACT/ARCON1,PREXP1,CR1,ARCON2,PREXP2,CR2,MODER              COMGEN    9
      COMMON/DROPL/EVAP(192),NTP4,NFNZ,XO(3),YO(3),ZO(3),ALFA(3),         COMGEN   10
     1  BETA(3),DELTA(3),THETA1(3),THETA2(3),NSL(3),WFF(3),SMD(3),        COMGEN   11
     2  VFUEL(3),RFUEL(3),EVSU(64),HEVAP                                  COMGEN   12
      COMMON/INJEC/FLOWIN,IUINJ(20),JUINJ(20),UINJ(20),WUINJ(20),         COMGEN   13
     1  AUINJ(20),TUINJ(20),IVINJ(20),JVINJ(20),KVINJ(20),VINJ(20),       COMGEN   14
     2  EVINJ(20),DVINJ(20),AVINJ(20),TVINJ(20),NUINJ,NVINJ,JSW1,JSW2,    COMGEN   15
     3  USW,VSW,AFSW,FSW,TSW,WSW,SWNO,RHOSW                               COMGEN   16
      COMMON/CSOOT/NVN,NVS1,NVS2,ISOOT,SSOOT,NSOOT,AO,ARCONN,AAA,BBB,FMG  SOOT      8
     1,GO,MPART,DPART(2),FRACP(2),RHOP,ARCONS,PREXPS,ALPHA,AAS,BBS,DHR    SOOT      9
     2,LVN,LVS1,LVS2,CINCP,TINCP,FUTOT                                    SOOT     10
      COMMON/CRAD/IRAD,SRAD                                               SOOT     11
      COMMON/CFOUP/PREXP3,ARCON3,CR3,PREXP4,ARCON4,CR4,AA1,BB1,CC1,       4STEP    15
     1 AA2,BB2,CC2,AA3,BB3,CC3,AA4,BB4,CC4,RATIO5,RATIO6,RATIO7,          4STEP    16
     2 RATIO8,RATIO9,RATO10,RATO11,RATO12,WCH,WH2,WC2H2,LVCH,LVCH1,LVH21  4STEP    17
      COMMON/CHDK/FDK(192)                                                NOX     146
      DIMENSION GENR(500),SUFU(500),SPFU(500),EDK2(192)                   NOX     147
      DIMENSION SUCH(500),SPCH(500)                                       4STEP   178
C *-*-*-*-*-*-*-*-*-*-  BEWARE OF EQUIVALENCE STATEMENTS  *-*-*-*-*-*-*-*-  AU        7
      EQUIVALENCE (GENR(1),DU(1)),(SUFU(1),DV(1)),(SPFU(1),DW(1))         AU        8
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C +-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-   AU          9
      ENTRY DENS                                                               AU         10
C-----ENTRY DENS IS USED TO CALCULATE TEMPERATURE AND DENSITY.                 COMMENT    72
C                                                                              COMMENT    73
      RELAXM=1.-RELAX(NRHO)                                                    AU         11
      KONTRO=2                                                                 AU         12
      IF(ISTEP.EQ.IRES)KONTRO=1                                                NASAX      28
      NVHP=7                                                                   AU         17
C-----ENTHALPY.                                                                COMMENT    74
      DO 1040 K=1,NP1                                                          AU         18
      DO 1040 J=1,MP1                                                          AU         19
      KJM=KM(K)+JM(J)                                                          AU         20
      DO 1040 I=1,LP1                                                          AU         21
      LP=KJM+I                                                                 AU         22
      LPH=LP+NVM(NVH)                                                          AU         23
      LPHP=LP+NVM(NVHP)                                                        AU         24
 1040 F(LPHP)=F(LPH)                                                           AU         25
      IF(ISOLVE(LVFU).EQ.0)GO TO 1034                                          NOX       148
      GO TO (1034,1044,1034), MODEN                                            AU         26
 1044 DO 1050 K=1,NP1                                                          AU         27
CALCULATE GAS TEMPERATURE.                                                     COMMENT    75
      DO 1050 J=2,M                                                            AU         28
      KJM=KM(K)+JM(J)                                                          AU         29
      IS=IWLI(J,4)                                                             AU         30
      IE=IWLO(J,4)                                                             AU         31
      DO 1050 I=IS,IE                                                          AU         32
      LP=KJM+I                                                                 AU         33
      LPHP=LP+NVM(NVHP)                                                        AU         34
      LPFU=LP+NVM(NVFU)                                                        AU         35
      LPCO=LP+NVM(NVCO)                                                        AU         36
      LPCH=LP+NVM(NVCH)                                                        4STEP     179
      LPH2=LP+NVM(NVH2)                                                        4STEP     180
      LPFUOX=LP+NVM(NVFUOX)                                                    AU         37
      T=TEMP(LP)                                                               AU         38
      F(LPFU)=AMIN1(F(LPFU),F(LPFUOX))                                         NOX       149
      FUB=F(LPFUOX)-F(LPFU)                                                    AU         39
      FLPCO2=WCO2*(CXX*FUB/WFU-CXX*F(LPCH)/WCH-F(LPCO)/WCO)                    4STEP     181
      FLPOX=RATIO1*F(LPFU)+RATIO3*F(LPCO)+RATIO2-(RATIO1+RATIO2)*              AU         41
     1 F(LPFUOX)+RATIO5*F(LPCH)+RATIO6*F(LPH2)                                 4STEP     182
      FLPOX=AMAX1(FLPOX,0.)                                                    AU         43
      FLPH2O=0.5*WH2O*(HYY*FUB/WFU-RATIO7*F(LPCH)-F(LPH2))                     4STEP     183
      FLPN2=1.0-F(LPFU)-FLPCO2-F(LPCO)-FLPOX-FLPH2O-F(LPCH)-F(LPH2)            4STEP     184
      FS(LP,IDFU)=F(LPFU)                                                      NOX       150
      FS(LP,IDO2)=AMIN1(FLPOX,RATIO2)                                          NOX       151
      FS(LP,IDN2)=AMAX1(1.E-15,FLPN2)                                          NOX       152
      FS(LP,IDCO)=F(LPCO)                                                      NOX       153
      FS(LP,IDCH)=F(LPCH)                                                      4STEP     185
      FS(LP,IDH2)=F(LPH2)                                                      4STEP     186
      FS(LP,IDH2O)=FLPH2O                                                      NOX       154
      FS(LP,IDCO2)=AMAX1(1.E-15,FLPCO2)                                        NOX       155
      IHCPS=4                                                                  NOX       156
      NS1=IDFU                                                                 NOX       157
      NS2=IDCO2                                                                NOX       158
      TK=T                                                                     NOX       159
      TKINV=1.0D0/TK                                                           NOX       160
      DO 1011 II=NS1,NS2                                                       NOX       161
 1011 S2(II)=FS(LP,II)/SMW(II)                                                 NOX       162
      CALL HCPS                                                                NOX       163
      HPI=HSUM*UNICON*TK                                                       NOX       164
      CPI=CPSUM*UNICON                                                         NOX       165
      T=TEMP(LP)+(F(LPHP)-HPI)/CPI                                             AU         50
      TEMP(LP)=(1.-RELAX(NVH))*TEMP(LP)+RELAX(NVH)*T                           AU         51
      PHI=F(LPFUOX)/FSTOIC                                                     AU         52
      TMAX=ACOEF(1)+PHI*(ACOEF(2)+PHI*(ACOEF(3)+PHI*ACOEF(4)))                 AU         53
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      TMAX=AMAX1(TMAX,2000.)                                            AU         54
      TEMP(LP)=AMIN1(TEMP(LP),TMAX)                                     AU         55
 1050 TEMP(LP)=AMAX1(TEMP(LP),100.)                                     AU         56
C -------- HERE DU IS U, DV IS V, DW IS W                              AU         57
 1034 REWIND NTP1                                                       AU         58
      READ (NTP1) DU,DV,DW,P                                            AU         59
 1048 READ (NTP1)                                                       AU         60
C -------- HERE PP IS PHI, DU IS MFU, DV IS MCO                        AU         61
      READ (NTP1) PP,DU,DV                                              AU         62
      READ(NTP1)                                                        RAD        32
      READ(NTP1)DW,P                                                    RAD        33
      REWIND NTP1                                                       AU         63
      READ(NTP1)U,V,W                                                   RAD        34
CALCULATE WALL TEMPERATURE.                                             COMMENT    76
      DO 1052 K=2,N                                                     RAD        35
      DO 1058 I=2,L                                                     RAD        36
      IF(IKIN(I,K).EQ.2.OR.IKIN(I,K).EQ.3)GO TO 1054                    RAD        37
      J=JWLO(I,4)-1                                                     RAD        38
      LP=I+JM(J)+KM(K)                                                  RAD        39
      LPRY=LP+NVM(5)                                                    RAD        40
      VEC=0.25*((U(LP)+U(LP+1))**2+(W(LP)+W(LP+NINJ))**2)               RAD        41
      HTC=CFR*RHO(LP)*CP*SQRT(VEC)                                      RAD        42
      TEMP(LP+NI)=TSOLVE(TEMP(LP+NI),TEMP(LP),F(LPRY),HTC,SIGMA,EMI,    RAD        43
     1 ITRAD)                                                           RAD        44
C                                                                       FEB2        2
 1054 IF(IKIN(I,K).EQ.1.OR.IKIN(I,K).EQ.3)GO TO 1056                    RAD        46
      IF(IDW.EQ.0)GO TO 1056                                            RAD        47
      J=JWLI(I,4)+1                                                     RAD        48
      LP=I+JM(J)+KM(K)                                                  RAD        49
      LPRY=LP+NVM(5)                                                    RAD        50
      VEC=0.25*((U(LP)+U(LP+1))**2+(W(LP)+W(LP+NINJ))**2)               RAD        51
      HTC=CFR*RHO(LP)*CP*SQRT(VEC)                                      RAD        52
      TEMP(LP-NI)=TSOLVE(TEMP(LP-NI),TEMP(LP),F(LPRY),HTC,SIGMA,EMI,    RAD        53
     1 ITRAD)                                                           RAD        54
 1056 CONTINUE                                                          RAD        55
      DO 1052 J=2,M                                                     RAD        56
      IF(JKIN(J,K).EQ.1)GO TO 1059                                      RAD        57
      LP=IWLI(J,4)+JM(J)+KM(K)                                          RAD        58
      LPRX=LP+NVM(10)                                                   RAD        59
      VEC=0.25*((V(LP)+V(LP+NI))**2+(W(LP)+W(LP+NINJ))**2)              RAD        60
      HTC=CFR*RHO(LP)*CP*SQRT(VEC)                                      RAD        61
      TEMP(LP-1)=TSOLVE(TEMP(LP-1),TEMP(LP),F(LPRX),HTC,SIGMA,EMI,ITRAD) RAD        62
 1059 IF(J.GT.JWOI.AND.J.LT.JWOO)GO TO 1052                             RAD        63
      LP=IWLO(J,4)+JM(J)+KM(K)                                          RAD        64
      LPRX=LP+NVM(10)                                                   RAD        65
      VEC=0.25*((V(LP)+V(LP+NI))**2+(W(LP)+W(LP+NINJ))**2)              RAD        66
      HTC=CFR*RHO(LP)*CP*SQRT(VEC)                                      RAD        67
      TEMP(LP+1)=TSOLVE(TEMP(LP+1),TEMP(LP),F(LPRX),HTC,SIGMA,EMI,ITRAD) RAD        68
 1052 CONTINUE                                                          RAD        69
      REWIND NTP1                                                       RAD        70
      READ(NTP1)U,V,W,P                                                 RAD        71
      IF(ISOLVE(LVFU).EQ.0)GO TO 1200                                   MOM       166
      GO TO (1060,1062,1064), MODEN                                     AU         65
 1060 DO 1061 K=1,KP1                                                   AU         66
C------DENSITY=CONSTANT.  MODEN=1.                                     COMMENT    77
      DO 1061 J=1,MP1                                                   AU         67
      KJM=KM(K)+JM(J)                                                   AU         68
      IS=IWLI(J,5)                                                      AU         69
      IE=IWLO(J,5)                                                      AU         70
      DO 1061 I=IS,IE                                                   AU         71
      LP=KJM+I                                                          AU         72
      RHO(LP)=DEN                                                       AU         73
 1061 CONTINUE                                                          AU         74
      GO TO 1200                                                        AU         75
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 1062 DO 1063 K=1,NP1                                                          AU      76
C-----DENSITY=FUNCTION(COMPOSITION,TEMPERATURE),  MODEN=2.                     COMMENT 78
      DO 1063 J=1,MP1                                                         AU      77
      KJM=KM(K)+JM(J)                                                         AU      78
      IS=IWLI(J,5)                                                            AU      79
      IE=IWLC(J,5)                                                            AU      80
      DO 1063 I=IS,IE                                                         AU      81
      LP=KJM+I                                                                AU      82
      LPTE=LP+NVM(NVTE)                                                       AU      83
      LPFUOX=LP+NVM(NVFUOX)                                                   AU      84
C  -----   CAUTION HERE                                                       AU      85
      LPFU=LP+NVM(NVFU+3)                                                     AU      86
      LPCO=LP+NVM(NVCO+1)                                                     AU      87
      LPCH=LP+NVM(NVCH)                                                       4STEP   187
      LPH2=LP+NVM(NVH2)                                                       4STEP   188
      FUR=F(LPFUOX)-F(LPFU)                                                   AU      88
      FLPH2O=0.5*WH2O*(HYY*FUR/WFU-RATIO7*F(LPCH)-F(LPH2))                    4STEP   189
      FLPCO2=WCO2*(CXX*FUR/WFU-CXX*F(LPCH)/WCH-F(LPCO)/WCO)                   4STEP   190
      FLPOX=RATIO1*F(LPFU)+RATIO3*F(LPCO)+RATIO2-(RATIO2+RATIO1)*             AU      91
     1 F(LPFUOX)+RATIO5*F(LPCH)+RATIO6*F(LPH2)                                4STEP   191
      FLPOX=AMAX1(FLPOX,0.)                                                   AU      93
      FLPN2=1.0-F(LPFU)-FLPCO2-F(LPCO)-FLPOX-FLPH2O-F(LPCH)-F(LPH2)           4STEP   192
 1008 CONTINUE                                                                AU      95
      FLPTE=F(LPTE)                                                           AU      96
      FLPTE=AMAX1(FLPTE,100.)                                                 AU      97
      VMIX=F(LPFU)/WFU+FLPCO2/WCO2+F(LPCO)/WCO+FLPOX/WOX+FLPH2O/WH2O+         AU      98
     1 FLPN2/WN2+F(LPCH)/WCH+F(LPH2)/WH2                                      4STEP   193
      DENST=RHOCON/(VMIX*FLPTE)                                               AU      100
      GO TO (1009,1010),KONTRO                                                AU      101
 1009 RHO(LP)=DENST                                                           AU      102
 1010 RHO(LP)=RELAX(NRHO)*DENST+RELAXM*RHO(LP)                                AU      103
 1063 CONTINUE                                                                AU      104
 1064 CONTINUE                                                                AU      105
 1200 CONTINUE                                                                AU      106
      CALL DENMOD                                                             AU      107
      RETURN                                                                  AU      108
C  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  * AU      109
      ENTRY VISCC                                                             AU      110
C-----ENTRY VISCO IS USED TO CALCULATE THE EFFECTIVE VISCOSITY                 COMMENT 79
C     AND YPLUS AT WALL BOUNDARIES.                                           COMMENT 80
C                                                                             COMMENT 81
C -------- HERE DU IS KE, DV IS DISS                                         AU      111
      READ (NTP1) DU,DV                                                       AU      112
      RELAXM=1.-RELAX(NGAM)                                                   AU      113
      KONTRO=2                                                                AU      114
      IF (ISTEP.EQ.IRES) KONTRO=1                                             AU      115
      DO 2000 K=1,NP1                                                         AU      116
      DO 2000 J=2,M                                                           AU      117
      KJM=KM(K)+JM(J)                                                         AU      118
      IS=IWLI(J,4)                                                            AU      119
      IE=IWLC(J,4)                                                            AU      120
      DO 2000 I=IS,IE                                                         AU      121
      LP=KJM+I                                                                AU      122
      GO TO (2001,2002),MODEL                                                 AU      123
 2001 CONTINUE                                                                AU      124
C-----CONSTANT VISCOSITY,  MODEL=1,  LAMINAR.                                 COMMENT 82
      VISC(LP)=AMU                                                            AU      125
      GO TO 2000                                                              AU      126
 2002 CONTINUE                                                                AU      127
      LPK=LP+NVM(NVK+4)                                                       AU      128
      LPD=LP+NVM(NVD+4)                                                       AU      129
C-----VISCOSITY FROM K-E MODEL,  MODEL=2,  TURBULENT.                         COMMENT 83
      VISCOS=RHO(LP)*CD*F(LPK)**2/(F(LPD)+1.E-30)                             AU      130
      GO TO (2003,2004),KONTRO                                                AU      131
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 2003 VISC(LP)=VISCOS                                                    AU      192
 2004 VISC(LP)=RELAX(NGAM)*VISCOS+RELAXM*VISC(LP)                        AU      193
 2000 CONTINUE                                                           AU      194
C ------- CALCULATE YPLUS                                               AU      195
      DO 2020 K=1,NP1                                                    AU      196
      DO 2022 I=1,LP1                                                    AU      197
      J=JWLO(I,4)                                                        AU      198
      LP=KM(K)+JM(J)+I                                                   AU      199
      LPK=LP+NVM(NVK+4)                                                  AU      200
      DIST=.5*YDIF(J)                                                    AU      201
      IF (J.EQ.MP1) DIST=YDIF(MP1)                                       AU      202
      YPLUS=RHO(LP-NI)*SQRT(F(LPK-NI)*RTCO)*DIST/AMU                     AU      203
      VISC(LP)=YPLUS                                                     AU      204
      J=JWLI(I,4)                                                        AU      205
      LP=KM(K)+JM(J)+I                                                   AU      206
      LPK=LP+NVM(NVK+4)                                                  AU      207
      DIST=.5*YDIF(J+1)                                                  AU      208
      IF (J.EQ.1) DIST=YDIF(2)                                           AU      209
      YPLUS=RHO(LP+NI)*SQRT(F(LPK+NI)*RTCO)*DIST/AMU                     AU      210
      VISC(LP)=YPLUS                                                     AU      211
 2022 CONTINUE                                                           AU      212
      DO 2024 J=2,M                                                      AU      213
      I=IWLI(J,4)-1                                                      AU      214
      LP=KM(K)+JM(J)+I                                                   AU      215
      LPK=LP+NVM(NVK+4)                                                  AU      216
      DIST=.5*XDIF(I+1)                                                  AU      217
      IF (I.EQ.1) DIST=XDIF(2)                                           AU      218
      YPLUS=RHO(LP+1)*SQRT(F(LPK+1)*RTCO)*DIST/AMU                       AU      219
      VISC(LP)=YPLUS                                                     AU      220
      I=IWLO(J,4)+1                                                      AU      221
      LP=KM(K)+JM(J)+I                                                   AU      222
      LPK=LP+NVM(NVK+4)                                                  AU      223
      DIST=.5*XDIF(I)                                                    AU      224
      IF (I.EQ.LP1) DIST=XDIF(LP1)                                       AU      225
      YPLUS=RHO(LP-1)*SQRT(F(LPK-1)*RTCO)*DIST/AMU                       AU      226
      VISC(LP)=YPLUS                                                     AU      227
 2024 CONTINUE                                                           AU      228
 2020 CONTINUE                                                           AU      229
      DO 3005 K=2,N                                                      AU      230
      DO 3005 J=2,M                                                      AU      231
      KJM=KM(K)+JM(J)                                                    AU      232
      IS=IWLI(J,4)                                                       AU      233
      IE=IWLO(J,4)                                                       AU      234
      DO 3005 I=IS,IE                                                    AU      235
      LP=KJM+I                                                           AU      236
      LPK=LP+NVM(NVK+4)                                                  AU      237
      LPD=LP+NVM(NVD+4)                                                  AU      238
      LPC=I-1+(J-2)*(NI-2)+(K-2)*(NI-2)*(NJ-2)                           AU      239
      EDK2(LPC)=F(LPD)/(F(LPK)**2+1.0E-30)                               SOOT    185
 3005 EDK(LPC)=F(LPD)/(F(LPK)+1.E-30)                                    AU      240
      RETURN                                                             AU      241
C  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  *  AU      242
      ENTRY GAMMA                                                        AU      243
C-----ENTRY GAMMA IS USED TO CALCULATE THE DIFFUSION COEFFICIENTS.       COMMENT  84
C                                                                        COMMENT  85
      DO 3000 K=1,NP1                                                    AU      244
      DO 3000 J=2,M                                                      AU      245
      KJM=KM(K)+JM(J)                                                    AU      246
      IS=IWLI(J,4)                                                       AU      247
      IE=IWLO(J,4)                                                       AU      248
      DO 3000 I=IS,IE                                                    AU      249
      LP=KJM+I                                                           AU      250
      GO TO (3001,3002),MODEL                                            AU      251
 3001 CONTINUE                                                           AU      252
188
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      GAM(LP)=VISC(LP)/PR(NV)                                              AU        193
      GO TO 3000                                                           AU        194
 3002 CONTINUE                                                             AU        195
      GAM(LP)=VISC(LP)/PREF(NV)                                            AU        196
 3000 CONTINUE                                                             AU        197
      CALL GAMOD                                                           AU        198
 3004 CONTINUE                                                             AU        199
      RETURN                                                               AU        200
C  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  * AU        201
      ENTRY SOURCE                                                         AU        202
C-----ENTRY SOURCE IS USED TO CALCULATE THE SOURCE TERMS FOR               COMMENT    86
C     THE DEPENDENT VARIABLES.                                             COMMENT    87
C                                                                          COMMENT    88
CAUTION NOT ALL SOURCE TERMS ARE VALID - AT BOUNDARY NODES -               AU        203
CHECK AND MODIFY ACCORDINGLY IN SOMOD                                      AU        204
      GO TO (100,200,300,400),NGOTO                                        AU        205
C +-+-+-+-+-+-+-+-    SOURCE TERMS FOR U-VELOCITY    +-+-+-+-+-+-+-+-+-+-  AU        206
100   DO 101 J=2,M                                                         AU        207
      IS=IWLI(J,NGOTO)                                                     AU        208
      IE=IWLO(J,NGOTO)                                                     AU        209
      DO 101 I=IS,IE                                                       AU        210
      LIJ=JM(J)+I                                                          AU        211
      LP=LIJ+KM(K)                                                         AU        212
      LXP=LP+1                                                             AU        213
      LXM=LP-1                                                             AU        214
      DUDXP=(U(LXP)-U(LP))/XS(I)                                           AU        215
      DUDXM=(U(LP)-U(LXM))/XS(I-1)                                         AU        216
      GAMLP=GAM(LP)                                                        AU        217
      GAMLXM=GAM(LXM)                                                      AU        218
      IF (I.EQ.IS) GAMLXM=GAM(LXM-1)                                       AU        219
      IF (I.EQ.IE) GAMLP=GAM(LP+1)                                         AU        220
      SU(LIJ)=(GAMLP*DUDXP-GAMLXM*DUDXM)/XSU(I)                            AU        221
      LYP=LP+NI                                                            AU        222
      LYM=LP-NI                                                            AU        223
      LYP1=LYP-1                                                           AU        224
      LYM1=LYM-1                                                           AU        225
      GAMP=0.25*(GAM(LP)+GAM(LXM)+GAM(LYP)+GAM(LYP1))                      AU        226
      GAMM=0.25*(GAM(LP)+GAM(LXM)+GAM(LYM)+GAM(LYM1))                      AU        227
      DVDXP=(V(LYP)-V(LYP1))/XDIF(I)                                       AU        228
      DVDXM=(V(LP)-V(LXM))/XDIF(I)                                         AU        229
      SU(LIJ)=SU(LIJ)+(GAMP*DVDXP*RM(J+1)-GAMM*DVDXM*RM(J))/YSR(J)         AU        230
      LZP=LP+NINJ                                                          AU        231
      LZM=LP-NINJ                                                          AU        232
      LZP1=LZP-1                                                           AU        233
      LZM1=LZM-1                                                           AU        234
      GAMP=0.25*(GAM(LP)+GAM(LXM)+GAM(LZP)+GAM(LZP1))                      AU        235
      GAMM=0.25*(GAM(LP)+GAM(LXM)+GAM(LZM)+GAM(LZM1))                      AU        236
      DWDXP=(W(LZP)-W(LZP1))/XDIF(I)                                       AU        237
      DWDXM=(W(LP)-W(LXM))/XDIF(I)                                         AU        238
      SU(LIJ)=SU(LIJ)+(GAMP*DWDXP-GAMM*DWDXM)*YS(J)/YSR(J)/ZS(K)           AU        239
      SP(LIJ)=0.                                                           AU        240
101   CONTINUE                                                             AU        241
      GO TO 5000                                                           AU        242
C +-+-+-+-+-+-+-+-    SOURCE TERMS FOR V-VELOCITY    +-+-+-+-+-+-+-+-+-+-  AU        243
200   DO 201 J=3,M                                                         AU        244
      IS=IWLI(J,NGOTO)                                                     AU        245
      IE=IWLO(J,NGOTO)                                                     AU        24
      DO 201 I=IS,IE                                                       AU        247
      LIJ=JM(J)+I                                                          AU        248
      LP=LIJ+KM(K)                                                         AU        249
      LYP=LP+NI                                                            AU        250
      LYM=LP-NI                                                            AU        251
      DVDYP=(V(LYP)-V(LP))/YS(J)                                           AU        252
      DVDYM=(V(LP)-V(LYM))/YS(J-1)                                         AU        253
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```
      GAMLP=GAM(LP)                                                     AU       254
      GAMLYM=GAM(LYM)                                                   AU       255
      IF (J.EQ.JWLI(I,NGOTO)+1) GAMLYM=GAM(LYM-NI)                      AU       256
      IF (J.EQ.JWLO(I,NGOTO)-1) GAMLP=GAM(LP+NI)                        AU       257
      SU(LIJ)=(GAMLP*DVDYP*RMV(J+1)-GAMLYM*DVDYM*RMV(J))/YSVR(J)        AU       258
      LXP=LP+1                                                          AU       259
      LXM=LP-1                                                          AU       260
      LXP1=LXP-NI                                                       AU       261
      LXM1=LXM-NI                                                       AU       262
      GAMP=0.25*(GAM(LP)+GAM(LYM)+GAM(LXP)+GAM(LXP1))                   AU       263
      GAMM=0.25*(GAM(LP)+GAM(LYM)+GAM(LXM)+GAM(LXM1))                   AU       264
      DUDYP=(U(LXP)-U(LXP1))/YDIF(J)                                    AU       265
      DUDYM=(U(LP)-U(LYM))/YDIF(J)                                      AU       266
      SU(LIJ)=SU(LIJ)+(GAMP*DUDYP-GAMM*DUDYM)/XS(I)                     AU       267
      LZP=LP+NINJ                                                       AU       268
      LZM=LP-NINJ                                                       AU       269
      LZP1=LZP-NI                                                       AU       270
      LZM1=LZM-NI                                                       AU       271
      GAMP=0.25*(GAM(LP)+GAM(LYM)+GAM(LZP)+GAM(LZP1))                   AU       272
      GAMM=0.25*(GAM(LP)+GAM(LYM)+GAM(LZM)+GAM(LZM1))                   AU       273
      DWDYP=(W(LZP)-W(LZP1))/YDIF(J)                                    AU       274
      DWDYM=(W(LP)-W(LYM))/YDIF(J)                                      AU       275
      SU(LIJ)=SU(LIJ)+(GAMP*DWDYP-GAMM*DWDYM)*YSV(J)/YSVR(J)/ZS(K)      AU       276
      WMNM=0.5*(W(LP)+W(LYM))                                           AU       277
      WMNP=0.5*(W(LZP)+W(LZP1))                                         AU       278
      SU(LIJ)=SU(LIJ)+PLAXM1*(GAMM*WMNM-GAMP*WMNP)*YSV(J)/YSVR(J)/ZS(K)/ AU      279
     1RM(J)                                                             AU       280
      GAMPT2=GAM(LP)+GAM(LYM)                                           AU       281
      SU(LIJ)=SU(LIJ)+PLAXM1*GAMPT2*(WMNM-WMNP)/RM(J)/ZS(K)/RM(J)       AU       282
      SP(LIJ)=-GAMPT2/RM(J)/RM(J)*PLAXM1                                AU       283
201   CONTINUE                                                          AU       284
      GO TO 5000                                                        AU       285
C +-+-+-+-+-+-+-+-+-    SOURCE TERMS FOR W-VELOCITY     +-+-+-+-+-+-+-+-+-+- AU       286
300   DO 301 J=2,M                                                      AU       287
      IS=IWLI(J,NGOTO)                                                  AU       288
      IE=IWLO(J,NGOTO)                                                  AU       289
      DO 301 I=IS,IE                                                    AU       290
      LIJ=JM(J)+I                                                       AU       291
      LP=LIJ+KM(K)                                                      AU       292
      LZP=LP+NINJ                                                       AU       293
      IF (K.EQ.NP1) LZP=LIJ+KM(3)                                       AU       294
      LZM=LP-NINJ                                                       AU       295
      DWDZP=(W(LZP)-W(LP))/ZS(K)                                        AU       296
      DWDZM=(W(LP)-W(LZM))/ZS(K-1)                                      AU       297
      GAMLP=GAM(LP)                                                     AU       298
      GAMLZM=GAM(LZM)                                                   AU       299
      IF(K.EQ.3) GAMLZM=GAM(LZM-NINJ)                                   AU       300
      SU(LIJ)=(GAMLP*DWDZP-GAMLZM*DWDZM)/R(J) /YSR(J)/ZSW(K)*YS(J)      AU       301
      LXP=LP+1                                                          AU       302
      LXM=LP-1                                                          AU       303
      LXP1=LXP-NINJ                                                     AU       304
      LXM1=LXP-NINJ                                                     AU       305
      GAMP=0.25*(GAM(LP)+GAM(LZM)+GAM(LXP)+GAM(LXP1))                   AU       306
      GAMM=0.25*(GAM(LP)+GAM(LZM)+GAM(LXM)+GAM(LXM1))                   AU       307
      DUDZP=(U(LXP)-U(LXP1))/ZDIF(K)                                    AU       308
      DUDZM=(U(LP)-U(LZM))/ZDIF(K)                                      AU       309
      SU(LIJ)=SU(LIJ)+(GAMP*DUDZP-GAMM*DUDZM)/XS(I)/R(J)                AU       310
      LYP=LP+NI                                                         AU       311
      LYM=LP-NI                                                         AU       312
      LYP1=LYP-NINJ                                                     AU       313
      LYM1=LYM-NINJ                                                     AU       314
      GAMP=0.25*(GAM(LP)+GAM(LZM)+GAM(LYP)+GAM(LYP1))                   AU       315
      GAMM=0.25*(GAM(LP)+GAM(LZM)+GAM(LYM)+GAM(LYM1))                   AU       316
      DWDZP=(W(LYP)-W(LYP1))/ZDIF(K)                                    AU       317
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      DVDZM=(V(LP)-V(LZM))/ZDIF(K)                                      AU  318
      SU(LIJ)=SU(LIJ)+(GAMP*DVDZP-GAMM*DVDZM)/YSP(J)                    AU  319
      WMNM=0.5*(W(LP)+W(LYM))                                           AU  320
      WMNP=0.5*(W(LP)+W(LYP))                                           AU  321
      SU(LIJ)=SU(LIJ)+PLAXM1*(GAMM*WMNM-GAMP*WMNP)/YSR(J)               AU  322
      VPT2=V(LP)+V(LYP)                                                 AU  323
      VMT2=V(LZM)+V(LZM+NI)                                             AU  324
      SU(LIJ)=SU(LIJ)+PLAXM1*(GAM(LP)*VPT2-VMT2*GAM(LZM))*YS(J)/R(J)/   AU  325
     1YSR(J)/ZSW(K)                                                     AU  326
      GAMP=0.5*(GAM(LP)+GAM(LZM))                                       AU  327
      SU(LIJ)=SU(LIJ)+PLAXM1*GAMP/R(J)*((WMNP-WMNM)/YS(J)+0.5*(VPT2-VMT2 AU  328
     1)/R(J)/ZSW(K))                                                    AU  329
      SP(LIJ)=-GAMP/R(J)/R(J)*PLAXM1                                    AU  330
301   CONTINUE                                                          AU  331
      GO TO 5000                                                        AU  332
C +-+-+-+-+-+-+-  SOURCE TERMS FOR TURBULENT KINETIC ENERGY  +-+-+-+-+-+-+ AU  333
                                                                        AU  334
400   CONTINUE                                                          AU  335
      IF (NV.NE.LVK) GO TO 500                                          AU  336
      DO 401 J=2,M                                                      AU  337
      IS=IWLI(J,NGOTO)                                                  AU  338
      IE=IWLO(J,NGOTO)                                                  AU  339
      DO 401 I=IS,IE                                                    AU  340
      MIN=JWLI(I,NGOTO)+1                                               AU  341
      MAX=JWLO(I,NGOTO)-1                                               AU  342
      LIJ=JM(J)+I                                                       AU  343
      LP=LIJ+KM(K)                                                      AU  344
      LXP=LP+1                                                          AU  345
      LYP=LP+NI                                                         AU  346
      LZP=LP+NINJ                                                       AU  347
      LXM=LP-1                                                          AU  348
      LYM=LP-NI                                                         AU  349
      LZM=LP-NINJ                                                       AU  350
      LPPO=LYP+1                                                        AU  351
      LPMO=LYM+1                                                        AU  352
      LPOM=LZM+1                                                        AU  353
      LPOP=LZP+1                                                        AU  354
      LMPO=LXM+NI                                                       AU  355
      LOPP=LZP+NI                                                       AU  356
      LOPM=LZM+NI                                                       AU  357
      LMOP=LXM+NINJ                                                     AU  358
      LOMP=LYM+NINJ                                                     AU  359
 CALCULATE THE PRODUCTION TERM                                          AU  360
      DUIDXJ(1,1)=(U(LXP)-U(LP))/XS(I)                                  AU  361
      DUIDXJ(2,2)=(V(LYP)-V(LP))/YS(J)                                  AU  362
      DUIDXJ(3,3)=(W(LZP)-W(LP))/ZS(K)/R(J)                             AU  363
     1 +PLAXM1*0.5*(V(LP)+V(LYP))/R(J)                                  AU  364
      IF (I-IS) 411,412,411                                             AU  365
 411  VXM=0.5*(V(LXP)+V(LMPO))                                          AU  366
      WXM=0.5*(W(LXM)+W(LMOP))                                          AU  367
      XM=X(I-1)                                                         AU  368
      GO TO 413                                                         AU  369
 412  VXM=0.5*(V(LP)+V(LYP))                                            AU  370
      WXM=0.5*(W(LP)+W(LZP))                                            AU  371
      XM=X(I)                                                           AU  372
 413  IF (I-IE) 414,415,414                                             AU  373
 414  VXP=0.5*(V(LXP)+V(LPPO))                                          AU  374
      WXP=0.5*(W(LXP)+W(LPOP))                                          AU  375
      XP=X(I+1)                                                         AU  376
      GO TO 416                                                         AU  377
 415  VXP=0.5*(V(LP)+V(LYP))                                            AU  378
      WXP=0.5*(W(LP)+W(LZP))                                            AU  379
      XP=X(I)                                                           AU  380
 416  DX=XP-XM                                                          AU  381
      DUIDXJ(2,1)=(VXP-VXM)/DX
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      DUIDXJ(3,1)=(WXP-WXM)/DX                                          AU        382
      IF (J-MIN) 421,422,421                                            AU        383
421   WYM=0.5*(W(LYM)+W(LOMP))                                          AU        384
      UYM=.5*(U(LYM)+U(LPMO))                                           AU        385
      YM=Y(J-1)                                                         AU        386
      GO TO 423                                                         AU        387
422   WYM=0.5*(W(LP)+W(LZP))                                            AU        388
      UYM=0.5*(U(LP)+U(LXP))                                            AU        389
      YM=Y(J)                                                           AU        390
  423 IF (J-MAX) 424,425,424                                            AU        391
424   WYP=0.5*(W(LYP)+W(LOPP))                                          AU        392
      UYP=0.5*(U(LYP)+U(LPPO))                                          AU        393
      YP=Y(J+1)                                                         AU        394
      GO TO 426                                                         AU        395
425   WYP=0.5*(W(LP)+W(LZP))                                            AU        396
      UYP=0.5*(U(LP)+U(LXP))                                            AU        397
      YP=Y(J)                                                           AU        398
426   DY=YP-YM                                                          AU        399
      DUIDXJ(3,2)=(WYP-WYM)/DY-PLAXM1*0.5*(W(LP)+W(LZP))/R(J)           AU        400
      DUIDXJ(1,2)=(UYP-UYM)/DY                                          AU        401
      IF(K-2) 431,432,431                                               AU        402
431   UZM=0.5*(U(LZM)+U(LPOM))                                          AU        403
      VZM=0.5*(V(LZM)+V(LOPM))                                          AU        404
      ZM=Z(K-1)                                                         AU        405
      GO TO 433                                                         AU        406
432   UZM=0.5*(U(LP)+U(LXP))                                            AU        407
      VZM=0.5*(V(LP)+V(LYP))                                            AU        408
      ZM=Z(K)                                                           AU        409
433   IF(K-N) 434,435,434                                               AU        410
434   UZP=0.5*(U(LZP)+U(LPOP))                                          AU        411
      VZP=0.5*(V(LZP)+V(LOPP))                                          AU        412
      ZP=Z(K+1)                                                         AU        413
      GO TO 436                                                         AU        414
435   UZP=0.5*(U(LP)+U(LXP))                                            AU        415
      VZP=0.5*(V(LP)+V(LYP))                                            AU        416
      ZP=Z(K)                                                           AU        417
436   DZ=ZP-ZM                                                          AU        418
      DUIDXJ(1,3)=(UZP-UZM)/DZ/R(J)                                     AU        419
      DUIDXJ(2,3)=(VZP-VZM)/DZ/R(J)                                     AU        420
      SUM=0.                                                            AU        421
      DO 402 II=1,3                                                     AU        422
      DO 402 JJ=1,3                                                     AU        423
402   SUM=SUM+(DUIDXJ(II,JJ)+DUIDXJ(JJ,II))*DUIDXJ(II,JJ)              AU        424
      GENR(LP)=SUM                                                      AU        425
CALCULATE THE SOURCE TERM                                               AU        426
      LPK=LP+NVM(NVK)                                                   AU        427
      LPO=LP+NVM(NVO)                                                   AU        428
      SU(LIJ)=RHO(LP)*CD*F(LPK)**2/(F(LPO)+1.E-30)*SUM                  AU        429
      SP(LIJ)=-RHO(LP)*F(LPO)/(F(LPK)+1.E-30)                           AU        430
C-----MODIFICATIONS OF THE SOURCE TERMS AT WALL BOUNDARIES.              COMMENT    89
      IF (I.GT.IS) GO TO 440                                            AU        431
      IF (JKIN(J,K).EQ.1) GO TO 440                                     AU        432
      DIST=.5*XDIF(I)                                                   AU        433
      IF (I.EQ.2) DIST=XDIF(2)                                          AU        434
      VP=.5*SQRT((V(LP)+V(LYP))**2+(W(LP)+W(LZP))**2)                   AU        435
      TAUP=AMAX1(GAM(LXM)*VP/DIST,1.E-20)                               AU        436
      GAM(LXM)=0.                                                       AU        437
      VXP=V(LP)+V(LYP)+V(LXP)+V(LPPO)                                   AU        438
      WXP=W(LP)+W(LZP)+W(LXP)+W(LPOP)                                   AU        439
      VC=.25*SQRT(VXP**2+WXP**2)                                        AU        440
      DVDY=VC/XS(I)                                                     AU        441
      SU(LIJ)=TAUP*DVDY                                                 AU        442
      SP(LIJ)=-RHO(LP)*RHO(LP)*CD*F(LPK)*DVDY/TAUP                      AU        443
  440 IF (I.LT.IE) GO TO 442                                            AU        444
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      IF (J.GT.JWOI.AND.J.LT.JWOO) GO TO 442                            AU      445
      DIST=.5*XDIF(I+1)                                                 AU      446
      IF (I.EQ.L) DIST=XDIF(LP1)                                        AU      447
      VP=.5*SQRT((V(LP)+V(LYP))**2+(W(LP)+W(LZP))**2)                   AU      448
      TAUP=AMAX1(GAM(LXP)*VP/DIST,1.E-20)                               AU      449
      GAM(LXP)=0.                                                       AU      450
      VXM=V(LP)+V(LYP)+V(LXM)+V(LMPO)                                   AU      451
      WXM=W(LP)+W(LZP)+W(LXM)+W(LMOP)                                   AU      452
      VC=.25*SQRT(VXM**2+WXM**2)                                        AU      453
      DVDY=VC/XS(I)                                                     AU      454
      SU(LIJ)=TAUP*DVDY                                                 AU      455
      SP(LIJ)=-RHO(LP)*RHO(LP)*CD*F(LPK)*DVDY/TAUP                      AU      456
  442 IF (J.GT.MIN) GO TO 444                                           AU      457
      IF (IOW.EQ.0.OR.IKIN(I,K).EQ.1.OR.IKIN(I,K).EQ.3) GO TO 444       AU      458
      DIST=.5*YDIF(J)                                                   AU      459
      IF (J.EQ.2) DIST=YDIF(2)                                          AU      460
      VP=.5*SQRT((U(LP)+U(LXP))**2+(W(LP)+W(LZP))**2)                   AU      461
      TAUP=AMAX1(GAM(LYP)*VP/DIST,1.E-20)                               AU      462
      GAM(LYP)=0.                                                       AU      463
      UYP=U(LP)+U(LXP)+U(LYP)+U(LPPO)                                   AU      464
      WYP=W(LP)+W(LZP)+W(LYP)+W(LOPP)                                   AU      465
      VC=.25*SQRT(UYP**2+WYP**2)                                        AU      466
      DVDY=VC/YS(J)                                                     AU      467
      SU(LIJ)=TAUP*DVDY                                                 AU      468
      SP(LIJ)=-RHO(LP)*RHO(LP)*CD*F(LPK)*DVDY/TAUP                      AU      469
  444 IF (J.LT.MAX) GO TO 401                                           AU      470
      IF (IKIN(I,K).EQ.2.OR.IKIN(I,K).EQ.3) GO TO 401                   AU      471
      DIST=.5*YDIF(J+1)                                                 AU      472
      IF (J.EQ.M) DIST=YDIF(MP1)                                        AU      473
      VP=.5*SQRT((U(LP)+U(LXP))**2+(W(LP)+W(LZP))**2)                   AU      474
      TAUP=AMAX1(GAM(LYP)*VP/DIST,1.E-20)                               AU      475
      GAM(LYP)=0.                                                       AU      476
      UYM=U(LP)+U(LXP)+U(LYM)+U(LPMO)                                   AU      477
      WYM=W(LP)+W(LZP)+W(LYM)+W(LOMP)                                   AU      478
      VC=.25*SQRT(UYM**2+WYM**2)                                        AU      479
      DVDY=VC/YS(J)                                                     AU      480
      SU(LIJ)=TAUP*DVDY                                                 AU      481
      SP(LIJ)=-RHO(LP)*RHO(LP)*CD*F(LPK)*DVDY/TAUP                      AU      482
401   CONTINUE                                                          AU      483
      GO TO 5000                                                        AU      484
C +-+-+-+-+-+-+-   SOURCE TERMS FOR TURBULENCE DISSIPATION  +-+-+-+-+-+-+-  AU      485
500   CONTINUE                                                          AU      486
      IF (NV.NE.LVD) GO TO 600                                          AU      487
      DO 501 J=2,M                                                      AU      488
      IS=IWLI(J,NGOTO)                                                  AU      489
      IE=IWLO(J,NGOTO)                                                  AU      490
      DO 501 I=IS,IE                                                    AU      491
      LIJ=JM(J)+I                                                       AU      492
      LP=LIJ+KM(K)                                                      AU      493
      LPK=LP+NVM(NVK)                                                   AU      494
      LPD=LP+NVM(NVD)                                                   AU      495
      SU(LIJ)=C1*CD*RHO(LP)*F(LPK)*GENR(LP)                             AU      496
      SP(LIJ)=-C2*RHO(LP)*F(LPD)/(F(LPK)+1.E-30)                        AU      497
501   CONTINUE                                                          AU      498
      GO TO 5000                                                        AU      499
C +-+-+-+-+-+-+-+-+-+-+-   SOURCE TERMS FOR FUEL   +-+-+-+-+-+-+-+-+-+-+-+  AU      500
600   CONTINUE                                                          AU      501
      IF (NV.NE.LVFU) GO TO 700                                         AU      502
      DO 601 J=2,M                                                      AU      503
      IS=IWLI(J,NGOTO)                                                  AU      504
      IE=IWLO(J,NGOTO)                                                  AU      505
      DO 601 I=IS,IE                                                    AU      506
      LIJ=JM(J)+I                                                       AU      507
      LP=LIJ+KM(K)                                                      AU      508
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      LPC=I-1+(J-2)*(NI-2)+(K-KSTR)*(NI-2)*(NJ-2)                        AU      509
      LPFU=LP+NVM(NVFU)                                                  AU      510
      LPFUOX=LP+NVM(NVFUOX)                                              AU      511
      LPCH=LP+NVM(NVCH)                                                  4STEP   194
      LPH2=LP+NVM(NVH2)                                                  4STEP   195
      LPTE=LP+NVM(NVTE)                                                  AU      512
      FLPTE=F(LPTE)                                                      AU      513
      FLPTE=AMAX1(FLPTE,100.)                                            AU      514
      F(LPFU)=AMIN1(F(LPFU),F(LPFUOX))                                   AU      515
      LPCO=LP+NVM(NVCO)                                                  AU      516
      FLPOX=RATIO1*F(LPFU)+RATIO3*F(LPCO)+RATIO2-(RATIO2+RATIO1)*        AU      517
     1 F(LPFUOX)+RATIO5*F(LPCH)+RATIO6*F(LPH2)                           4STEP   196
      FLPOX=AMAX1(FLPOX,0.)                                              AU      519
      RHOLP=ABS(RHO(LP))                                                 AU      520
      ARRHEN=-PREXP1*EXP(-ARCON1/FLPTE)                                  4STEP   197
      SOR1=((F(LPFU)*RHOLP)**AA1)*((FLPOX*RHOLP)**BB1)*((F(LPCH)*RHOLP)  4STEP   198
     1**CC1)*ARRHEN                                                      4STEP   199
      GO TO (611,612),MODER                                              AU      522
  611 SOR=SOR1                                                           AU      523
      GO TO 602                                                          AU      524
  612 LPK=LP+NVM(NVK)                                                    AU      525
      LPD=LP+NVM(NVD)                                                    AU      526
      PHI=F(LPFU)                                                        4STEP   200
      SOR2=-CR1*PHI*RHO(LP)*EDK(LPC)                                     AU      528
      SOR=AMAX1(SOR1,SOR2)                                               AU      529
  602 FUB=AMAX1(0.,((RATIO2+RATIO1)*F(LPFUOX)-RATIO2-RATIO3*F(LPCO)      4STEP   201
     1-RATIO5*F(LPCH)-RATIO6*F(LPH2))/RATIO1)                            4STEP   202
      FUB=AMIN1(F(LPFU),FUB)                                             4STEP   203
      DSDFU=SOR/(F(LPFU)-FUB+1.E-30)                                     4STEP   204
      SU(LIJ)=SOR-DSDFU*F(LPFU)                                          AU      534
      SP(LIJ)=DSDFU                                                      AU      535
      SUFU(LP)=SU(LIJ)                                                   AU      536
      SPFU(LP)=SP(LIJ)                                                   AU      537
  601 CONTINUE                                                           AU      538
      GO TO 5000                                                         AU      539
C +-+-+-+-+-+-+-+-+-+-+-+-+-   SOURCE TERMS FOR ENTHALPY   +-+-+-+-+-+-+-+-+-+-+-+-+-  AU      540
  700 CONTINUE                                                           AU      541
      IF (NV.NE.LVH) GO TO 800                                           AU      542
      DO 701 J=2,M                                                       AU      543
      IS=IVLI(J,NGOTO)                                                   AU      544
      IF=IVLO(J,NGOTO)                                                   AU      545
      DO 701 I=IS,IF                                                     AU      546
      LIJ=JM(J)+I                                                        AU      547
      SU(LIJ)=0.                                                         AU      548
      SP(LIJ)=0.                                                         AU      549
      IF(ITRAD.EQ.1)GO TO 701                                            RAD      72
      LP=LIJ+KM(K)                                                       AU      552
      LPH=LP+NVM(NVH)                                                    AU      553
      LPFAV=LP+NVM(NVFAV)                                                AU      554
      LPTE=LP+NVM(NVTE)                                                  AU      555
      FLPTE=F(LPTE)                                                      AU      556
      FLPE=SIGMA*FLPTE**4                                                AU      557
      FAV=F(LPFAV)                                                       AU      558
      SOR=6.0*ABSR(LP)*(FAV-FLPE)                                        RAD      73
      TO=(FAV/SIGMA)**.25                                                AU      560
      TO=TO+.001                                                         AU      561
      DSDH=SOR/(CP*(FLPTE-TO))                                           AU      562
      SU(LIJ)=SU(LIJ)+SOR-DSDH*F(LPH)                                    AU      563
      SP(LIJ)=SP(LIJ)+DSDH                                               AU      564
  701 CONTINUE                                                           AU      565
      GO TO 5000                                                         AU      566
C -+-+-+-+-+-+-+-+-+-+-+-+-+  SOURCE TERMS FOR PHI  +-+-+-+-+-+-+-+-+-+-+-+-+  AU      567
  800 CONTINUE                                                           AU      568
      IF (NV.NE.LVFUOX) GO TO 900                                        AU      569
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      DO 801 J=2,M                                                      AU        570
      IS=IWLI(J,NGCTO)                                                  AU        571
      IE=IWLO(J,NGCTO)                                                  AU        572
      DO 801 I=IS,IE                                                    AU        573
      LIJ=JM(J)+I                                                       AU        574
      SU(LIJ)=0.                                                        AU        575
      SP(LIJ)=0.                                                        AU        576
801   CONTINUE                                                          AU        577
      GO TO 5000                                                        AU        578
C-+-+-+-+-+-+-+-+-+-+-+-+-     SOURCE TERM FOR CO      +-+-+-+-+-+-+-+-+-+-+-+ +-+ AU        579
  900 IF(NV.NE.LVCO)GO TO 950                                           4STEP     205
      SFAC=2.48*(1.0-FSTOIC)/FSTOIC                                     4STEP     206
      DO 901 J=2,M                                                      AU        581
      IS=IWLI(J,NGCTO)                                                  AU        582
      IE=IWLO(J,NGCTO)                                                  AU        583
      DO 901 I=IS,IE                                                    AU        584
      LIJ=JM(J)+I                                                       AU        585
      LP=LIJ+KM(K)                                                      AU        586
      LPC=I-1+(J-2)*(NI-2)+(K-KSTR)*(NI-2)*(NJ-2)                       AU        587
      LPCO=LP+NVM(NVCO)                                                 AU        588
      LPFUOX=LP+NVM(NVFUOX)                                             AU        589
      LPFU=LP+NVM(NVFU)                                                 AU        590
      LPTE=LP+NVM(NVTE)                                                 AU        591
      LPCH=LP+NVM(NVCH)                                                 4STEP     207
      LPH2=LP+NVM(NVH2)                                                 4STEP     208
      FLPTE=F(LPTE)                                                     AU        592
      FLPTE=AMAX1(FLPTE,100.)                                           AU        593
      FLPOX=RATIO1*F(LPFU)+RATIO3*F(LPCO)+RATIO2-(RATIO2+RATIO1)*       AU        594
     1 F(LPFUOX)+RATIO5*F(LPCH)+RATIO6*F(LPH2)                          4STEP     209
      FLPOX=AMAX1(FLPOX,0.)                                             AU        595
      FUB=F(LPFUOX)-F(LPFU)                                             4STEP     210
      FLPH2O=0.5*WH2O*(HYY*FUB/WFU-RATIO7*F(LPCH)-F(LPH2))              4STEP     211
      FLPH2O=AMAX1(0.0,FLPH2O)                                          4STEP     212
      RHOLP=APS(RHO(LP))                                                4STEP     213
      ARRHEN=-PREXP3*EXP(-ARCON3/FLPTE)                                 4STEP     214
      SOR3=((F(LPCO)*RHOLP)**AA3)*((FLPOX*RHOLP)**BB3)*((FLPH2O*RHOLP)  4STEP     215
     1**CC3)*ARRHEN                                                     4STEP     216
      SSS=7.93*EXP(-F(LPFUOX)*SFAC/(1.0-F(LPFUOX)))                     4STEP     217
      SSS=AMIN1(SSS,1.0)                                                4STEP     218
      SOR3=SOR3*SSS                                                     4STEP     219
      GO TO (911,912),MODER                                             AU        599
  911 SORCO=SOR3                                                        AU        600
      GO TO 902                                                         AU        601
  912 CONTINUE                                                          AU        602
      PHI=AMIN1(F(LPCO),FLPOX/RATIO3)                                   AU        603
      SOR4=-CR3*PHI*RHO(LP)*EDK(LPC)                                    4STEP     220
      SORCO=AMAX1(SOR3,SOR4)                                            AU        605
  902 FUB=AMAX1(0.,((RATIO2+RATIO1)*F(LPFUOX)-RATIO2-RATIO1*F(LPFU)     4STEP     221
     1-RATIO5*F(LPCH)-RATIO6*F(LPH2))/RATIO3)                           4STEP     222
      FUB=AMIN1(F(LPCO),FUB)                                            4STEP     223
      DSDCO=SORCO/(F(LPCO)-FUB+1.E-30)                                  4STEP     224
      SU(LIJ)=SORCO-DSDCO*F(LPCO)-RATIO11*(SUCH(LP)+SPCH(LP)*F(LPCH))   4STEP     225
      SP(LIJ)=DSDCO                                                     AU        611
  901 CONTINUE                                                          AU        612
      GO TO 5000                                                        4STEP     226
  950 IF(NV.NE.LVCH)GO TO 960                                           4STEP     227
C-----SOURCE TERMS FOR CHMY-2---------------------------------------    4STEP     228
      DO 951 J=2,M                                                      4STEP     229
      IS=IWLI(J,NGCTO)                                                  4STEP     230
      IE=IWLO(J,NGCTO)                                                  4STEP     231
      DO 951 I=IS,IE                                                    4STEP     232
      LIJ=JM(J)+I                                                       4STEP     233
      LP=LIJ+KM(K)                                                      4STEP     234
      LPC=I-1+(J-2)*(NI-2)+(K-KSTR)*(NI-2)*(NJ-2)                       4STEP     235
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      LPCO=LP+NVM(NVCO)                                                 4STEP     236
      LPFUOX=LP+NVM(NVFUOX)                                             4STEP     237
      LPFU=LP+NVM(NVFU)                                                 4STEP     238
      LPTE=LP+NVM(NVTE)                                                 4STEP     239
      LPCH=LP+NVM(NVCH)                                                 4STEP     240
      LPH2=LP+NVM(NVH2)                                                 4STEP     241
      FLPTE=F(LPTE)                                                     4STEP     242
      FLPTE=AMAX1(FLPTE,100.)                                           4STEP     243
      FLPOX=RATIO1*F(LPFU)+RATIO3*F(LPCO)+RATIO2-(RATIO2+RATIO1)*       4STEP     244
     1 F(LPFUOX)+RATIO5*F(LPCH)+RATIO6*F(LPH2)                          4STEP     245
      FLPOX=AMAX1(FLPOX,0.0)                                            4STEP     246
      ARRHEN=-PREXP2*EXP(-ARCON2/FLPTE)                                 4STEP     247
      RHOLP=ABS(RHO(LP))                                                4STEP     248
      SOR1=((F(LPCH)*RHOLP)**AA2)*((FLPOX*RHOLP)**BB2)*((F(LPFU)*RHOLP  4STEP     249
     1+1.E-30)**CC2)*ARRHEN                                             4STEP     250
      IF(MODER.EQ.2)GO TO 952                                           4STEP     251
      SOR=SOR1                                                          4STEP     252
      GO TO 953                                                         4STEP     253
  952 PHI=AMIN1(F(LPCH),FLPOX/RATIO5)                                   4STEP     254
      SOR2=-CR2*PHI*RHO(LP)*EDK(LPC)                                    4STEP     255
      SOR=AMAX1(SOR1,SOR2)                                              4STEP     256
  953 FUB=AMAX1(0.,((RATIO2+RATIO1)*F(LPFUOX)-RATIO2-RATIO3*F(LPCO)     4STEP     257
     1-RATIO1*F(LPFU)-RATIO6*F(LPH2))/RATIO5)                           4STEP     258
      FUR=AMIN1(F(LPCH),FUB)                                            4STEP     259
      DSDSP=SOR/(F(LPCH)-FUR+1.E-30)                                    4STEP     260
      SUCH(LP)=SOR-DSDSP*F(LPCH)                                        4STEP     261
      SPCH(LP)=DSDSP                                                    4STEP     262
      SU(LIJ)=SUCH(LP)-RATIO8*(SUFU(LP)+SPFU(LP)*F(LPFU))               4STEP     263
      SP(LIJ)=DSDSP                                                     4STEP     264
  951 CONTINUE                                                          4STEP     265
      GO TO 9000                                                        4STEP     266
  960 IF(NV.NE.LVH2)GO TO 1000                                          4STEP     267
C-----SOURCE TERMS FOR H2---------------------------------------------- 4STEP     268
      DO 961 J=2,M                                                      4STEP     269
      IS=IWLI(J,NGOTO)                                                  4STEP     270
      IF=IWLO(J,NGOTO)                                                  4STEP     271
      DO 961 I=IS,IF                                                    4STEP     272
      LIJ=JM(J)+I                                                       4STEP     273
      LP=LIJ-KM(K)                                                      4STEP     274
      LPC=I-1+(J-2)*(NI-2)+(K-KSTR)*(NI-2)*(MJ-2)                       4STEP     275
      LPCO=LP+NVM(NVCO)                                                 4STEP     276
      LPFUOX=LP+NVM(NVFUOX)                                             4STEP     277
      LPFU=LP+NVM(NVFU)                                                 4STEP     278
      LPTE=LP+NVM(NVTE)                                                 4STEP     279
      LPCH=LP+NVM(NVCH)                                                 4STEP     280
      LPH2=LP+NVM(NVH2)                                                 4STEP     281
      FLPTE=F(LPTE)                                                     4STEP     282
      FLPTE=AMAX1(FLPTE,100.)                                           4STEP     283
      FLPOX=RATIO1*F(LPFU)+RATIO3*F(LPCO)+RATIO2-(RATIO2+RATIO1)*       4STEP     284
     1 F(LPFUOX)+RATIO5*F(LPCH)+RATIO6*F(LPH2)                          4STEP     285
      FLPOX=AMAX1(FLPOX,0.0)                                            4STEP     286
      ARRHEN=-PREXP4*EXP(-ARCON4/FLPTE)                                 4STEP     287
      RHOLP=ABS(RHO(LP))                                                4STEP     288
      SOR1=((F(LPH2)*RHOLP)**AA4)*((FLPOX*RHOLP)**BB4)*((F(LPCH)*RHOLP  4STEP     289
     1+1.E-30)**CC4)*ARRHEN                                             4STEP     290
      IF(MODER.EQ.2)GO TO 962                                           4STEP     291
      SOR=SOR1                                                          4STEP     292
      GO TO 963                                                         4STEP     293
  962 PHI=AMIN1(F(LPH2),FLPOX/RATIO6)                                   4STEP     294
      SOR2=-CR4*PHI*RHO(LP)*EDK(LPC)                                    4STEP     295
      SOR=AMAX1(SOR1,SOR2)                                              4STEP     296
  963 FUR=AMAX1(0.,((RATIO2+RATIO1)*F(LPFUOX)-RATIO2-RATIO3*F(LPCO)     4STEP     297
     1-RATIO1*F(LPFU)-RATIO5*F(LPCH))/RATIO6)                           4STEP     298
      FUR=AMIN1(F(LPH2),FUR)                                            4STEP     299
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      DSDSP=SUR/(F(LPH2)-FUR+1.E-30)                                    4STEP    300
      SU(LIJ)=SOR-DSDSP*F(LPH2)-RATO12*(SUFU(LP)+SPFU(LP)*F(LPFU))      4STEP    301
     1-RATO10*(SUCH(LP)+SPCH(LP)*F(LPCH))                               4STEP    302
      SP(LIJ)=DSDSP                                                     4STEP    303
  961 CONTINUE                                                          4STEP    304
      GO TO 5000                                                        SOOT     187
C+-+-+-+-+-+-+-+-  SOURCE TERM FOR NUCLEI CONCENTRATION  +-+-+-+-+-+-+-+-+ SOOT     188
 1000 IF(NV.NE.LVN)GO TO 1100                                           SOOT     189
      DO 1001 J=2,M                                                     SOOT     190
      IS=IWLI(J,NGOTO)                                                  SOOT     191
      IE=IWLO(J,NGOTO)                                                  SOOT     192
      DO 1001 I=IS,IE                                                   SOOT     193
      LIJ=JM(J)+I                                                       SOOT     194
      LP=LIJ+KM(K)                                                      SOOT     195
      LPFUOX=LP+NVM(NVFUOX)                                             SOOT     196
      LPFU=LP+NVM(NVFU)                                                 SOOT     197
      LPCO=LP+NVM(NVCO)                                                 SOOT     198
      LPTE=LP+NVM(NVTE)                                                 SOOT     199
      LPCH=LP+NVM(NVCH)                                                 4STEP    305
      LPH2=LP+NVM(NVH2)                                                 4STEP    306
      T=F(LPTE)                                                         SOOT     200
      FLPOX=RATIO1*F(LPFU)+RATIO3*F(LPCO)+RATIO2-(RATIO2+RATIO1)*       SOOT     201
     1 F(LPFUOX)+RATIO7*F(LPCH)+RATIO6*F(LPH2)                          4STEP    307
      FLPOX=AMAX1(FLPOX,1.E-30)                                         SOOT     203
      CARB=F(LPFUOX)*12.0*CXX/WFU                                       SOOT     204
      LPC=I-1+(J-2)*(NI-2)+(K-KSTR)*(NI-2)*(NJ-2)                       SOOT     205
      LPS1=LP+NVM(NVS1)                                                 SOOT     206
      LPS2=LP+NVM(NVS2)                                                 SOOT     207
      LPN=LP+NVM(NVN)                                                   SOOT     208
      FUR=F(LPFUOX)-F(LPFU)                                             SOOT     209
      FLPCO2=WCO2*(CXX*FUR/WFU-CXX*F(LPCH)/WCH-F(LPCO)/WCO)             4STEP    308
      FLPH20=0.5*WH20*(HYY*FUR/WFU-RATIO7*F(LPCH)-F(LPH2))              4STEP    309
      FLPN2=1.0-F(LPFU)-FLPCO2-F(LPCO)-FLPOX-FLPH20-F(LPCH)-F(LPH2)     4STEP    310
      VMIX=F(LPFU)/WFU+FLPCO2/WCO2+F(LPCO)/WCO+FLPOX/WOX+FLPH20/WH20    SOOT     213
     1+FLPN2/WN2+F(LPCH)/WCH+F(LPH2)/WH2                                4STEP    311
      RET=(ANU*EDK2(LPC)/RHO(LP))**0.25                                 SOOT     215
      EMDOT=23.6*RET*EDK(LPC)                                           SOOT     216
      EMPR=FUR*(1.0+RATIO1)                                             SOOT     217
      PSI=EMPR/(EMPR+F(LPFU)+(1.0+RATIO1))                              SOOT     218
      EMMIN=AMIN1(F(LPFU),FLPOX/RATIO1)                                 SOOT     219
C-----BYPASS CALCULATION IF TEMP.LT.TINCP, OR IF                        COMMENT   90
C     CARBON/OXYGEN RATIO LT.CINCP (TINCP AND CINCP INPUT BY USER).     COMMENT   91
      IF(T.LT.TINCP)GO TO 1006                                          SOOT     220
      IF(CARB/FLPOX.LT.CINCP)GO TO 1006                                 SOOT     221
      EMP=(F(LPS1)/DPART(1)**3+F(LPS2)/(DPART(2)+1.E-30)**3)            SOOT     222
     1/(F(LPS1)+F(LPS2))                                                SOOT     223
      EMP=RHOP*3.14159/(6.0*EMP)                                        SOOT     224
      AND=AO*RHO(LP)*F(LPFU)*EXP(-ARCONN/F(LPTE))                       SOOT     225
      GAMAS=AMIN1(1.0,9.7*RET**3)                                       SOOT     226
      GPSI=GAMAS*PSI                                                    SOOT     227
      OGPSI=1.0-GPSI                                                    SOOT     228
      IHCPS=1                                                           NOX      167
      NS1=IOFU                                                          NOX      168
      NS2=IOCO2                                                         NOX      169
C-----CALCULATE MIXTURE CP.                                             COMMENT   92
      TK=T                                                              NOX      170
      TKINV=1.000/TK                                                    NOX      171
      DO 1012 II=NS1,NS2                                                NOX      172
 1012 S2(II)=FS(LP,II)/SMW(II)                                          NOX      173
      CALL HCPS                                                         NOX      174
      CPR=CPSUM*UNICON                                                  NOX      175
      DELTAT=DHR*EMPIN/CPR                                              SOOT     231
      TSTR=F(LPTE)+DELTAT                                               SOOT     232
      RHOSTR=RHOCON/(VMIX*TSTR)                                         SOOT     233
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      TO=F(LPTE)-DELTAT*GPSI/DGPSI                                          SOOT      284
      TO=AMAX1(TO,100.0)                                                    SOOT      285
      RHOO=RHOCON/(VMIX*TO)                                                 SOOT      286
      ANOSTR=AO*RHOSTR*F(LPFU)*EXP(-ARCONN/TSTR)                            SOOT      287
      ANOO=AO*RHOO*F(LPFU)*EXP(-ARCONN/TO)                                  SOOT      288
      GPSIR=GPSI/RHOSTR                                                     SOOT      289
      DGPSIR=DGPSI/RHOO                                                     SOOT      290
      ENRHO=F(LPN)/RHO(LP)                                                  SOOT      291
      EMDOTR=EMDOT*RHOSTR/(GPSI*DGPSI)                                      SOOT      292
      ENN=(F(LPS1)+F(LPS2))*RHO(LP)/EMP                                     SOOT      293
      ENNRHO=ENN/RHO(LP)                                                    SOOT      294
      A1=(ANOSTR+EMDOTR*ENRHO)/GO                                           SOOT      295
      A2=(FMG-EMDOTR/RHOSTR)/GO                                             SOOT      296
      A3=EMDOTR*A1/RHOSTR                                                   SOOT      297
      A4=EMDOTR*(A2/RHOSTR-ENNRHO)                                          SOOT      298
      A5=-BBB*A1                                                            SOOT      299
      A6=AAA-BBB*A2                                                         SOOT      300
      ARG=SQRT(ABS((A4-A5)**2+4.0*A6*A3))                                   SOOT      301
      ENSTR1=(A4-A5+ARG)/(2.0*A6)                                           SOOT      302
      ENSTR2=(A4-A5-ARG)/(2.0*A6)                                           SOOT      303
      ENSTR=ENSTR1                                                          SOOT      304
      IF(ENSTR1.LT.0.0)ENSTR=ENSTR2                                         SOOT      305
      ENSTR=AMIN1(ENSTR,ENRHO/GPSIR)                                        SOOT      306
      ENSTR=AMAX1(ENSTR,ENRHO*RHOSTR)                                       SOOT      307
      ENSTR=AMAX1(1.0,ENSTR)                                                SOOT      308
      ENNSTR=(A1+A2*ENSTR)/ENSTR                                            SOOT      309
      ENNSTR=AMIN1(ENNSTR,AAA/BBB)                                          SOOT      310
      ENNSTR=AMIN1(ENNSTR,ENNRHO/GPSIR)                                     SOOT      311
      ENNSTR=AMAX1(1.0,ENNSTR)                                              SOOT      312
      ENO=(ENRHO-ENSTR*GPSIR)/DGPSIR                                        SOOT      313
      ENO=AMAX1(1.0,ENO)                                                    SOOT      314
      ENNO=(ENNRHO-ENNSTR*GPSIR)/DGPSIR                                     SOOT      315
      ENNO=AMAX1(1.0,ENNO)                                                  SOOT      316
      FMGF=FMG*F(LPN)                                                       SOOT      317
      SUF1=ANO+FMGF                                                         SOOT      318
      SPF1=GO*ENN                                                           SOOT      319
      SUF2=(ANOSTR*GPSIR+ANOO*DGPSIR+GO*ENSTR*GPSIR*(ENNO-ENNSTR))          SOOT      320
     1*RHO(LP)+FMGF                                                         SOOT      321
      SPF2=GO*ENNO                                                          SOOT      322
      RF1=SUF1-SPF1*F(LPN)                                                  SOOT      323
      RF2=SUF2-SPF2*F(LPN)                                                  SOOT      324
C-----FORMATION RATE.                                                       COMMENT    93
      IF(RF1.GT.RF2)GO TO 1004                                              SOOT      325
      SU(LIJ)=SUF1                                                          SOOT      326
      SP(LIJ)=-SPF1                                                         SOOT      327
      GO TO 1005                                                            SOOT      328
 1004 SU(LIJ)=SUF2                                                          SOOT      329
      SP(LIJ)=-SPF2                                                         SOOT      330
      GO TO 1005                                                            SOOT      331
 1004 SU(LIJ)=0.0                                                           SOOT      332
      SP(LIJ)=0.0                                                           SOOT      333
C-----OXIDATION RATE.                                                       COMMENT    94
 1005 RNC=EMDOT*PSI*EMPIN/(F(LPFU)+1.E-30)                                  SOOT      334
      SP(LIJ)=SP(LIJ)-RNC                                                   SOOT      335
 1001 CONTINUE                                                              SOOT      336
      GO TO 9000                                                            SOOT      337
C+-+-+-+-+-+-+-+-  SOURCE TERM FOR SOOT CONCENTRATION  +-+-+-+-+-+-+-+-+-+ SOOT      338
 1100 IF(NV.LT.LVS1.OR.NV.GT.LVS2)GO TO 1300                                SOOT      339
      II=NV-LVS1+1                                                          SOOT      340
      CONS2=6.0/(RHOP*DPART(II))                                            SOOT      341
      DO 1101 J=2,M                                                         SOOT      342
      IS=IWLI(J,NGOTO)                                                      SOOT      343
      IE=IWLC(J,NGOTO)                                                      SOOT      344
      DO 1101 I=IS,IE                                                       SOOT      345
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      LIJ=JM(J)+I                                                       SOOT     296
      LP=LIJ+KM(K)                                                      SOOT     297
      LPFUOX=LP+NVM(NVFUOX)                                             SOOT     298
      LPFU=LP+NVM(NVFU)                                                 SOOT     299
      LPCO=LP+NVM(NVCO)                                                 SOOT     300
      LPTE=LP+NVP(NVTE)                                                 SOOT     301
      LPCH=LP+NVM(NVCH)                                                 4STEP    312
      LPH2=LP+NVM(NVH2)                                                 4STEP    313
      T=F(LPTE)                                                         SOOT     302
      FLPOX=RATIO1*F(LPFU)+RATIO3*F(LPCO)+RATIO2-(RATIO2+RATIO1)*       SOOT     303
     1 F(LPFUOX)+RATIO5*F(LPCH)+RATIO6*F(LPH2)                          4STEP    314
      FLPOX=AMAX1(FLPOX,1.E-30)                                         SOOT     305
      CARB=F(LPFUOX)*12.0*CXX/WFU                                       SOOT     306
      LPC=I-1+(J-2)*(NI-2)+(K-KSTR)*(NI-2)*(NJ-2)                       SOOT     307
      LPS1=LP+NVM(NVS1)                                                 SOOT     308
      LPS2=LP+NVM(NVS2)                                                 SOOT     309
      LPS=LP+NVM(NV)                                                    SOOT     310
      LPN=LP+NVM(NVN)                                                   SOOT     311
      FUB=F(LPFUOX)-F(LPFU)                                             SOOT     312
      FLPCO2=WCO2*(CXX*FUB/WFU-CXX*F(LPCH)/WCH-F(LPCO)/WCO)             4STEP    315
      FLPH2O=0.5*WH2O*(HYY*FUB/WFU-RATIO7*F(LPCH)-F(LPH2))              4STEP    316
      FLPN2=1.0-F(LPFU)-FLPCO2-F(LPCO)-FLPOX-FLPH2O-F(LPCH)-F(LPH2)     4STEP    317
      VMIX=F(LPFU)/WFU+FLPCO2/WCO2+F(LPCO)/WCO+FLPOX/WOX+FLPH2O/WH2O    SOOT     318
     1+FLPN2/WN2+F(LPCH)/WCH+F(LPH2)/WH2                                4STEP    318
      RET=(ANU*EDK2(LPC)/RHO(LP))**0.25                                 SOOT     319
      EMDOT=23.6*RET*EDK(LPC)                                           SOOT     320
      EMPR=FUB*(1.0+RATIO1)                                             SOOT     321
      PSI=EMPR/(EPPR+F(LPFU)*(1.0+RATIO1))                              SOOT     322
      FMMIN=AMIN1(F(LPFU),FLPOX/RATIO1)                                 COMMENT   95
C-----BYPASS CALCULATION IF TEMP.LT.TINCP, OR IF                        COMMENT   96
C     CARBON/OXYGEN RATIO LT.CINCP (TINCP AND CINCP INPUT BY USER).     SOOT     323
      IF(T.LT.TINCP)GO TO 1106                                          SOOT     324
      IF(CARB/FLPOX.LT.CINCP)GO TO 1106                                 SOOT     325
      EMP=(F(LPS1)/DPART(1)**3+F(LPS2)/(DPART(2)*1.E-30)**3)            SOOT     326
     1/(F(LPS1)+F(LPS2))                                                SOOT     327
      EMP=RHOP*3.14159/(6.0*EMP)                                        SOOT     328
      ANO=AO*RHO(LP)*F(LPFU)*EXP(-ARCONN/F(LPTE))                       SOOT     329
      GAMAS=AMIN1(1.0,9.7*RET**3)                                       SOOT     330
      GPSI=GAMAS*PSI                                                    SOOT     331
      OGPSI=1.0-GPSI                                                    NOX      176
      IHCPS=1                                                           NOX      177
      NS1=IOFU                                                          NOX      178
      NS2=IOCO2                                                         COMMENT   97
C-----CALCULATE MIXTURE CP.                                             NOX      179
      TK=T                                                              NOX      180
      TKINV=1.000/TK                                                    NOX      181
      DO 1013 II=NS1,NS2                                                NOX      182
 1013 S2(II)=FS(LP,II)/SMW(II)                                          NOX      183
      CALL HCPS                                                         NOX      184
      CPR=CPSUM*UNICON                                                  SOOT     334
      DELTAT=QHR*EMMIN/CPR                                              SOOT     335
      TSTR=F(LPTE)+DELTAT                                               SOOT     336
      RHOSTR=RHOCON/(VMIX*TSTR)                                         SOOT     337
      TO=F(LPTE)-DELTAT*GPSI/OGPSI                                      SOOT     338
      TO=AMAX1(TO,100.0)                                                SOOT     339
      RHOO=RHOCON/(VMIX*TO)                                             SOOT     340
      ANOSTR=AO*RHOSTR*F(LPFU)*EXP(-ARCONN/TSTR)                        SOOT     341
      ANOO=AO*RHOO*F(LPFU)*EXP(-ARCONN/TO)                              SOOT     342
      GPSIR=GPSI/RHOSTR                                                 SOOT     343
      OGPSTR=OGPSI/RHOO                                                 SOOT     344
      ENRHO=F(LPN)/RHO(LP)                                              SOOT     345
      EMDOTR=EMDOT*RHOSTR/GPSI                                          SOOT     346
      ENN=(F(LPS1)+F(LPS2))*RHO(LP)/EMP                                 SOOT     347
      ENNRHO=ENN/RHO(LP)
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      A1=(ANOSTR+ENDOTR*ENRHO)/GO                                          SOOT     348
      A2=(FMG-ENDOTR/RHOSTR)/GO                                            SOOT     349
      A3=ENDOTR*A1/RHOSTR                                                  SOOT     350
      A4=ENDOTR*(A2/RHOSTR-ENNRHO)                                         SOOT     351
      A5=-BBB*A1                                                           SOOT     352
      A6=AAA-BBB*A2                                                        SOOT     353
      ARG=SQRT(ABS((A4-A5)**2+4.0*A6*A3))                                  SOOT     354
      ENSTR1=(A4-A5+ARG)/(2.0*A6)                                          SOOT     355
      ENSTR2=(A4-A5-ARG)/(2.0*A6)                                          SOOT     356
      ENSTR=ENSTR1                                                         SOOT     357
      IF(ENSTR1.LT.C.0)ENSTR=ENSTR2                                        SOOT     358
      ENSTR=AMIN1(ENSTR,ENRHO/GPSIR)                                       SOOT     359
      ENSTR=AMAX1(ENSTR,ENRHO*RHOSTR)                                      SOOT     360
      ENSTR=AMAX1(1.0,ENSTR)                                               SOOT     361
      ENNSTR=(A1+A2*ENSTR)/ENSTR                                           SOOT     362
      ENNSTR=AMIN1(ENNSTR,AAA/BBB)                                         SOOT     363
      ENNSTR=AMIN1(ENNSTR,ENNRHO/GPSIR)                                    SOOT     364
      ENNSTR=AMAX1(1.0,ENNSTR)                                             SOOT     365
      ENO=(ENRHO-ENSTR*GPSIR)/DGPSIR                                       SOOT     366
      ENO=AMAX1(1.0,ENO)                                                   SOOT     367
      ENNO=(ENNRHO-ENNSTR*GPSIR)/DGPSIR                                    SOOT     368
      ENNO=AMAX1(1.0,ENNO)                                                 SOOT     369
C-----QUASIGLOBAL FORMATION RATE.                                          COMMENT   98
      SUF1=PREXPS*F(LPTE)**ALPHA*(RHO(LP)*F(LPFU))**AAS*(RHO(LP)*FLPOX)    SOOT     370
     1**BBS*EXP(-ARCONS/F(LPTE))*FRACP(II)                                 SOOT     371
C-----TURBULENT FORMATION RATE.                                            COMMENT   99
      SUF2=ENP*(AAA*F(LPN)+BBB*ENNSTR*GPSIR*RHO(LP)*(ENO-ENSTR))           SOOT     372
     1*FRACP(II)                                                           SOOT     373
      SPF2=RHO(LP)*BBB*ENO*FRACP(II)                                       SOOT     374
      SPF2F=SPF2*F(LPS)                                                    SOOT     375
      SUF2=AMAX1(SUF2,SPF2F)                                               SOOT     376
      RF2=SUF2-SPF2F                                                       SOOT     377
      IF(SUF1.GT.RF2)GO TO 1104                                            SOOT     378
      SU(LIJ)=SUF1                                                         SOOT     379
      SP(LIJ)=0.C                                                          SOOT     380
      GO TO 1105                                                           SOOT     381
 1104 SU(LIJ)=SUF2                                                         SOOT     382
      SP(LIJ)=-SPF2                                                        SOOT     383
      GO TO 1105                                                           SOOT     384
 1106 SU(LIJ)=0.C                                                          SOOT     385
      SP(LIJ)=0.0                                                          SOOT     386
C-----SURFACE OXIDATION RATE.                                              COMMENT  100
 1105 AREAT=CONS2*RHO(LP)                                                  SOOT     387
      AKA=2000.0*EXP(-15100./F(LPTE))                                      JAN14      1
      AKB=4.46E-1*EXP(-7640./F(LPTE))                                      JAN14      2
      AKZ=21.3*EXP(2060./F(LPTE))                                          SOOT     390
      AKT=1.51E6*EXP(-48800./F(LPTE))                                      SOOT     391
      PO2=FLPOX*PRESS/(VMIX*32.0*101325.0)                                 SOOT     392
      PSIC=1.0/(1.0+AKT/(AKB*PO2))                                         SOOT     393
      AKK=AKA*PO2/(1.0+AKZ*PO2)                                            SOOT     394
      SPC1=12.0*AREAT*(AKK*PSIC+AKB*PO2*(1.0-PSIC))                        SOOT     395
C-----TURBULENT OXIDATION RATE.                                            COMMENT  101
      SPC2=ENDOT*PSI*FMMIN*RHO(LP)/(F(LPFU)*1.E-30)                        SOOT     396
      SPC1=AMIN1(SPC1,SPC2)                                                SOOT     397
      SP(LIJ)=SP(LIJ)-SPC1                                                 SOOT     398
 1101 CONTINUE                                                             SOOT     399
      GO TO 5000                                                           SOOT     400
C+-+-+- OTHER SPECIES - H,O,OH,N,NO,NO2 -+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+  COMMENT  102
C       THESE SOURCES CALCULATED IN KINETICS PROGRAM CREK.                 COMMENT  103
C                                                                          COMMENT  104
 1300 IF(NV.NE.LVH1)GO TO 1400                                             NOX      185
      DO 1201 J=2,N                                                        NOX      186
      IS=IWLI(J,NGOTO)                                                     NOX      187
      IF=IWLO(J,NGOTO)                                                     NOX      188
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      DO 1201 I=IS,IE                                                    NOX      189
      LIJ=I+JP(J)                                                        NOX      190
      SU(LIJ)=0.0                                                        NOX      191
 1201 SP(LIJ)=0.0                                                        NOX      192
      GO TO 5000                                                         NOX      193
 1400 CONTINUE                                                           NOX      194
 5000 CONTINUE                                                           AU       615
      RETURN                                                             AU       616
      END                                                                AU       617
      SUBROUTINE AUXRAD                                                  AUR        2
      COMMON F(3500),DU(500),DV(500),DW(500),                            COMFB      2
     1 ANUC(500),SQOT1(500),SQOT2(500),FCH(500),FH2(500),FS(500,14),     4STEP     10
     1 RHO(500),VISC(500),ABSR(500),SCTR(500),SU(100),SP(100),           RAD        3
     1 DRHODP(500),                                                     RAD        4
     1  AXP(100),AXM(100),AYP(100),AYM(100),AZP(100),                   COMFB      4
     2  AZM(100),CZ(100),CY(10),CZU(100),CYU(10),                       COMFB      5
     3  CZP(100),CYP(10),DIV6(100),NTP1,NTP2                            COMFB      6
     1,AXMK(192),AXPK(192),AYMK(192),AYPK(192),AZMK(192),AZPK(192),      CTOMA      3
     2 SUK(192),SPK(192)                                                CTOMA      4
      DIMENSION U(500),V(500),W(500),PP(500),P(500),TEMP(500)            COMFB      7
      DIMENSION GAM(500)                                                 COMFB      8
      EQUIVALENCE (F(1),U(1)),(F(501),V(1)),(F(1001),W(1))               COMFB      9
      EQUIVALENCE (F(1501),PP(1)),(F(2001),P(1)),(F(2501),TEMP(1))       COMFB     10
      EQUIVALENCE (F(3001),GAM(1))                                       COMFB     11
      COMMON/CYL/R(30),RM(30),RMV(30),YSR(30),YSVR(30),IPLAX             COMMON     2
      COMMON/GRID/X(40),Y(30),Z(30),XS(40),YS(30),ZS(30),XSU(40),        COMMON     3
     1  YSV(30),ZSW(30),XDIF(40),YDIF(30),ZDIF(30),FXP(40),FXM(40),      COMMON     4
     2  FYP(30),FYM(30),FZP(30),FZM(30),DT,TIME                          COMMON     5
      COMMON                                                             NOX        2
     1/CINDEX/IDCO,IDFU,IO2,IDN2,IDH2O,IDCO2,IDH1,IDH2,IDN1,IDNO,IDNO2   NOX        3
     1,IDO,IDOH,IHCPS,ILC,ILH,INAT,ITER,JJJ,N1,N2,N3,NA,NGLOB,NGLOBP,    NOX        4
     2 NLM,NQ,NSP,NS1,NS2,IDCH                                           4STEP      3
     3/CCHEMI/CPSUP,HSUM,FQ,PPLN,RGAS,RGASIN,SMINV,TKINV,TLN,LNRG        NOX        6
     4/CPARAM/ASUB(30,3),EMV,ER,HSUBO,NDEBUG,NS,PA,QO,Q1,Q2,Q3,Q4,RHOPP, NOX        7
     4 SM,SMW(30),SPO,S1(30),S2(30),TK,LADIAB,LDEBUG,LEQUIL,LREACT,      NOX        8
     4 LENER,EDKIJ,LCONVG                                                NOX        9
      DOUBLE PRECISION CPSUM,EMV,ER,FQ,HSUBO,HSUM,PA,PPLN,QO,Q1,Q2,Q3,   NOX       10
     1 Q4,RGAS,RGASIN,RHOPP,SM,SMINV,SMW,S1,S2,TK,TKINV,TLN,SMO          NOX       11
     2,FUT,FST                                                           4STEP      4
      COMMON/STEP4/PEXP1,PEXP2,PEXP3,PEXP4,ER1,ER2,ER3,ER4,CEBU1,CEBU2,  4STEP      5
     1 CEBU3,CEBU4,AEXP1,AEXP2,AEXP3,AEXP4,BEXP1,BEXP2,BEXP3,BEXP4,      4STEP      6
     2 CEXP1,CEXP2,CEXP3,CEXP4,FUT,FST                                   4STEP      7
      LOGICAL LADIAB,LCONVG,LDEBUG,LEQUIL,LNRG,LREACT,LENER              NOX       12
      COMMON/INT/L,M,N,LCV,MCV,NCV,LP1,MP1,NP1,NI,NJ,NK,NINJ,NINJNK,NV,  COMMON     6
     1 NNV,NGOTO,K,ISTR,JSTR,KSTR,NVM(35),KM(30),JM(30),ISTEP,           4STEP      8
     2 ISOLVE(32),IPRINT(33),TITLE(10,33),IXY,ISWP,JSWP,RELAX(35),NP,    4STEP      9
     3  NRHO,NGAP,IWLI(30,5),IWLO(30,5),JWLO(40,5),JWLI(40,5),IWEI,      COMMON     9
     4  IWEO,MM1,JWII,JWIO,JWOI,JWOO,IDW,JKIN(30,30),IKIN(40,30)         COMMON    10
      COMMON/INDEX/IPAR,LPREF,ISTUN,INCOMP,ITRAD,NVRX,NVRY,NVRZ,JPLANE   COMMON    11
     1,PLAXM1,LVK,LVO,LVFUOX,LVFU,LVCO,LVH,LVRK,LVRY,LVRZ,NVF(32),       4STEP     10
     2  IJUMP,IRES,TITLE2(20),IMAX,JMAX,KMAX,NVCO,FUNCO,NVH2O,NVCO2,     COMMON    13
     3 NVN2,NVCH,NVH2                                                    4STEP     11
      COMMON/CNOX/LVH1,LVH2,LVN1,LVNO,LVNO2,LVO,LVOH,LVH2O,LVN2,LVO2,    NOX       16
     1 LVCO2,LVFU1,LVCO1,NNOX,INOX,ITNOX,SNOX,TNOX                       NOX       17
      COMMON/THERP/NVH,NVFU,NVOX,NVFUOX,NVTE,MODEN,IDK,FSTOIC,HFU,CP,    COMMON    15
     1  GASCON,RHOCON,UNICON,PRESS,NVFAV,TCYLW,TINLW,TLIP,ACOEF(4),      COMMON    16
     2  T4,DFAC,WFU,WCO2,WCO,WOX,WH2O,WN2,HYY,CXX,RATIO1,RATIO2,         COMMON    17
     3  RATIO3,RATIO4,HCO,TAN,ITWALL                                     COMMON    18
      COMMON/CTOMA/KEND,ICTOMA(32)                                       4STEP     12
      COMMON/MIS/AMU,DEN,SMAX,SSUM,LASTEP,HTCEXT,CFR,EMISW,EMISIN,       CONGEN     2
     1  EMISR,TOUT,RTCO,EMI,RADIN,RADSUR,FMA,FK,SOFK,                    CONGEN     3
     2  FKFU,FOFU,TFUEL,WFNZ,FLO(40),TEMTM(40),H(40),FUEL(40),FUOX(40) ,  CONGEN     4
     2 UIN(40),TIN(40),FUELS(40),SEXIT,IGAM1(29),IGAM2(29)               4STEP     13
      COMMON/TURB/NVK,NVO,C1,C2,CO,AK,DUIDXJ(3,3),AKFAC,ALFAC,           CONGEN     6
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     1 MODEL,PR(32),PREF(32),PJAY(32),E                                  4STEP    14
       COMMON/PAD/NVE,SIGMA,ABSOR,SCATR                                  COMGEN    8
       COMMON/REACT/ARCON1,PREXP1,CR1,ARCON2,PREXP2,CR2,MODER            COMGEN    9
       COMMON/DROPL/EVAP(192),NTP4,NFNZ,XD(3),YD(3),ZD(3),ALFA(3),       COMGEN   10
      1  BETA(3),DELTA(3),THETA1(3),THETA2(3),NSL(3),WFF(3),SMD(3),      COMGEN   11
      2  VFUEL(3),RFUEL(3),EVSU(64),HEVAP                                COMGEN   12
       COMMON/INJEC/FLOWIN,IUINJ(20),JUINJ(20),UINJ(20),WUINJ(20),       COMGEN   13
      1  AUINJ(20),TUINJ(20),IVINJ(20),JVINJ(20),KVINJ(20),VINJ(20),     COMGEN   14
      2  EVINJ(20),DVINJ(20),AVINJ(20),TVINJ(20),NUINJ,NVINJ,JSW1,JSW2,  COMGEN   15
      3  USW,VSW,AFSW,FSW,TSW,WSW,SWNO,RHOSW                             COMGEN   16
       COMMON/CSOOT/NVN,NVS1,NVS2,ISOOT,SSOOT,NSOOT,AO,ARCONN,AAA,BBB,FMG SOOT    8
      1,GO,MPART,DPART(2),FRACP(2),RHOP,ARCONS,PREXPS,ALPHA,AAS,BBS,DHR  SOOT    9
      2,LVN,LVS1,LVS2,CINCP,TINCP,FUTOT                                  SOOT   10
       COMMON/CRAD/IRAD,SRAD                                             SOOT   11
       COMMON/CFOUR/PREXP3,ARCON3,CR3,PREXP4,ARCON4,CR4,AA1,BB1,CC1,     4STEP   15
      1 AA2,BB2,CC2,AA3,BB3,CC3,AA4,BB4,CC4,RATIO5,RATIO6,RATIO7,        4STEP   16
      2 RATIO8,RATIO9,RATO10,RATO11,RATO12,WCH,WH2,WC2H4,LVCH,LVCH1,LVH21 4STEP   17
C  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  AUR      6
       ENTRY GAMRAD                                                      AUR      7
C-----ENTRY GAMRAD IS USED TO CALCULATE THE GAMAS IN THE RADIATION        COMMENT  105
C      EQUATIONS.                                                        COMMENT  106
C                                                                        COMMENT  107
       IF (NV.EQ.LVRY) GO TO 3100                                        AUR      8
       DO 4002 K=1,NP1                                                   RAD     74
       DO 4002 J=1,NP1                                                   RAD     75
       KJM=KM(K)+JP(J)                                                   RAD     76
       IS=IWLI(J,4)                                                      RAD     77
       IE=IWLO(J,4)                                                      RAD     78
       DO 4002 I=IS,IE                                                   RAD     79
       LP=KJM+I                                                          RAD     80
C-----VALUES OF ABSORPTION AND SCATTERING COEFFICIENTS FOR                COMMENT  108
C      ITRAD=2.                                                          COMMENT  109
       ABSR(LP)=ABSOR                                                    RAD     81
 4002 SCTR(LP)=SCATR                                                     RAD     82
       IF(ITRAD.NE.3)GO TO 4001                                          RAD     83
C-----ABSORPTION COEFFICIENT CALCULATED FROM SUBROUTINE ABSOR             COMMENT  110
C      (ITRAD=3).                                                        COMMENT  111
       DO 4000 K=2,N                                                     RAD     84
       DO 4000 J=2,M                                                     RAD     85
       KJM=KM(K)+JP(J)                                                   RAD     86
       IS=IWLI(J,4)                                                      RAD     87
       IE=IWLO(J,4)                                                      RAD     88
       DO 4000 I=IS,IE                                                   RAD     89
       LP=KJM+I                                                          RAD     90
       TS=TEMP(LP)                                                       RAD     91
       TS=AMAX1(TS,300.0)                                                RAD     92
       TS=AMIN1(TS,2000.0)                                               RAD     93
       T=TS                                                              RAD     94
       PATH=2.0*Y(MP1)                                                   RAD     95
C-----SOOT CONCENTRATION.                                                COMMENT  112
       SOOTK=7.0*(SOOT1(LP)+SOOT2(LP))*RHO(LP)/(RHOP*0.94E-6)            RAD     96
       LPFU=LP+NVM(NVFU)                                                 RAD     97
       LPFUOX=LP+NVM(NVFUOX)                                             RAD     98
       LPCO=LP+NVM(NVCO)                                                 RAD     99
       LPCH=LP+NVM(NVCH)                                                 4STEP  319
       LPH2=LP+NVP(NVH2)                                                 4STEP  320
       FUR=F(LPFUOX)-F(LPFU)                                             RAD    100
C-----CO2 AND H2O CONCENTRATIONS.                                        COMMENT  113
       FLPCO2=WCO2*(CXX*FUR/WFU-CXX*F(LPCH)/WCH-F(LPCO)/WCO)             4STEP  321
       FLPCO2=AMAX1(1.E-30,FLPCO2)                                       RAD    102
       FLPOX=AMAX1(0.0,RATIO1*F(LPFU)+RATIO3*F(LPCO)+RATIO2              RAD    103
      1-(RATIO1+RATIO2)*F(LPFUOX)+RATIO5*F(LPCH)+RATIO6*F(LPH2))         4STEP  322
       FLPH2O=0.50*WH2O*(HYY*FUR/WFU-RATIO7*F(LPCH)-F(LPH2))             4STEP  323
       FLPH2O=AMAX1(1.E-30,FLPH2O)                                       RAD    106
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      FLPN2=1.0-F(LPFU)-FLPCO2-F(LPCO)-FLPOX-FLPH2O-F(LPCH)-F(LPH2)      4STEP    324
      FLPN2=AMAX1(0.0,FLPN2)                                             RAD      108
      VMIX=F(LPFU)/WFU+FLPCO2/WCO2+F(LPCO)/WCO+FLPOX/WOX+FLPH2O/WH2O     RAD      109
     1+FLPN2/WN2+F(LPCH)/WCH+F(LPH2)/WH2                                 4STEP    325
      PCO2=FLPCO2/(VMIX*WCO2)                                            RAD      111
      PH2O=FLPH2O/(VMIX*WH2O)                                            RAD      112
      PCO2=AMIN1(PCO2,1.0-PH2O)                                          RAD      113
      FACP=5.97*T/TS                                                     RAD      114
      PATH=AMIN1(PATH,FACP/PCO2)                                         RAD      115
      PATH=AMIN1(PATH,FACP/PH2O)                                         RAD      116
      CALL ABSORB(TS,T,PATH,SOOTK,PCO2,PH2O,ALPHAS)                      RAD      117
      ALPHAS=AMIN1(ALPHAS,0.999)                                         RAD      118
      ABSR(LP)=-ALOG(1.0-ALPHAS)/PATH                                    RAD      119
 4000 CONTINUE                                                           RAD      120
 4001 CONTINUE                                                           RAD      121
CALCULATE GAMA FOR X-DIRECTION FLUX.                                     COMMENT  114
      DO 3000 K=1,NP1                                                    AUR       9
      DO 3000 J=1,MP1                                                    AUR      10
      KJM=KM(K)+JM(J)                                                    AUR      11
      IS=IWLI(J,4)                                                       AUR      12
      IE=IWLO(J,4)                                                       AUR      13
      DO 3000 I=IS,IE                                                    AUR      14
      LP=KJM+I                                                           AUR      15
      GAM(LP)=1.0/(ABSR(LP)+SCTR(LP))                                    RAD      122
 3000 CONTINUE                                                           AUR      17
      GO TO 3300                                                         AUR      18
CALCULATE GAMA FOR Y-DIRECTION FLUX.                                     COMMENT  115
 3100 DO 3200 K=1,NP1                                                    AUR      19
      DO 3200 J=1,MP1                                                    AUR      20
      KJM=KM(K)+JM(J)                                                    AUR      21
      IS=IWLI(J,4)                                                       AUR      22
      IE=IWLO(J,4)                                                       AUR      23
      DO 3200 I=IS,IE                                                    AUR      24
      LP=KJM+I                                                           AUR      25
      GAM(LP)=1.0/(ABSR(LP)+SCTR(LP)+1.0/(R(J)+1.E-30))                  RAD      123
 3200 CONTINUE                                                           AUR      27
 3300 RETURN                                                             AUR      28
C  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  AUR      29
      ENTRY SORAD                                                        AUR      30
C-----ENTRY SORAD IS USED TO CALCULATE THE SOURCE TERMS IN THE           COMMENT  116
C     RADIATION EQUATIONS.                                               COMMENT  117
C                                                                        COMMENT  118
      IF (NV.EQ.LVR2) GO TO 300                                          AUR      31
C-----X- AND Y-DIRECTION FLUXES.                                         COMMENT  119
      DO 101 J=2,N                                                       AUR      32
      IS=IWLI(J,NGOTO)                                                   AUR      33
      IE=IWLO(J,NGOTO)                                                   AUR      34
      DO 101 I=IS,IE                                                     AUR      35
      LIJ=JM(J)+I                                                        AUR      36
      LP=LIJ+KM(K)                                                       AUR      37
      LPRX=LP+NVM(NVRX)                                                  AUR      38
      LPRY=LP+NVM(NVRY)                                                  AUR      39
      LPRZ=LP+NVM(NVRZ)                                                  AUR      40
      LPTE=LP+NVM(NVTE)                                                  AUR      41
      FLPTE=F(LPTE)                                                      AUR      42
      FLPE=SIGMA*FLPTE**4                                                AUR      43
      SU(LIJ)=ABSR(LP)*FLPE*SCTR(LP)*(F(LPRX)+F(LPRY)+F(LPRZ))/3.        RAD      124
      SP(LIJ)=-(ABSR(LP)+SCTR(LP))                                       RAD      125
  101 CONTINUE                                                           AUR      46
      RETURN                                                             AUR      47
  300 CONTINUE                                                           AUR      48
C-----Z-DIRECTION FLUX.                                                  COMMENT  120
      DO 301 K=2,N                                                       AUR      49
      KJM=KM(K)+JM(JPLANE)                                               AUR      50
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      IS=IWLI(JPLANE,NGOTO)                                              AUR        58
      IF=IWLO(JPLANE,NGOTO)                                              AUR        59
      DO 301 I=IS,IF                                                     AUR        60
      LIK=JM(K)+I                                                        AUR        61
      LP=KJM+I                                                           AUR        62
      LPRX=LP+NVM(NVRX)                                                  AUR        63
      LPRY=LP+NVM(NVRY)                                                  AUR        64
      LPRZ=LP+NVM(NVRZ)                                                  AUR        65
      LPTF=LP+NVM(NVTF)                                                  AUR        66
      FLPTE=F(LPTE)                                                      AUR        67
      FLPE=SIGMA*FLPTE**4                                                RAD       126
      SU(LIK)=ABSR(LP)*FLPE*SCTR(LP)*(F(LPRX)+F(LPRY)+F(LPRZ))/3.        RAD       127
      SP(LIK)=-(ABSR(LP)+SCTR(LP))                                       AUR        68
  301 CONTINUE                                                           AUR        69
      RETURN                                                             AUR        70
      END                                                                SP          2
      SUBROUTINE SPRAY                                                   SP          3
C ********************** SUBROUTINE SPRAY ***************************.***  SP          4
C     SUBROUTINE FOR AIRTRIP CODE WHICH CALCULATES THE TRAJECTORY        SP          5
C     AND EVAPORATION RATES FOR A FUEL NOZZLE SPRAY.  WRITTEN NOV. 1976  SP          6
C ***************************************************************************
      COMMON F(3500),DU(500),DV(500),DW(500),                            COMFB       2
     1 ANUC(500),SOOT1(500),SOOT2(500),FCH(500),FH2(500),FS(500,14),     4STEP      18
     1 RHO(500),VISC(500),ABSR(500),SCTR(500),SU(100),SP(100),           RAD         3
     1 DRHODP(500),                                                     RAD         4
     1  AXP(100),AXM(100),AYP(100),AYM(100),AZP(100),                   COMFB       4
     2  AZM(100),CZ(100),CY(10),CZU(100),CYU(10),                       COMFB       5
     3  CZP(100),CYP(10),DIVG(100),NTP1,NTP2                            COMFB       6
     1,AXMK(192),AXPK(192),AYMK(192),AYPK(192),AZMK(192),AZPK(192),      CTDMA       3
     2 SUK(192),SPK(192)                                                CTDMA       4
      DIMENSION U(500),V(500),W(500),PP(500),P(500),TEMP(500)           COMFB       7
      DIMENSION GAM(500)                                                COMFB       8
      EQUIVALENCE (F(1),U(1)),(F(501),V(1)),(F(1001),W(1))              COMFB       9
      EQUIVALENCE (F(1501),PP(1)),(F(2001),P(1)),(F(2501),TEMP(1))      COMFB      10
      EQUIVALENCE (F(3001),GAM(1))                                      COMFB      11
      COMMON/CYL/R(30),RM(30),RMV(30),YSR(30),YSVR(30),IPLAX            COMMON      2
      COMMON/GRID/X(40),Y(30),Z(30),XS(40),YS(30),ZS(30),XSU(40),       COMMON      3
     1  YSV(30),ZSW(30),XDIF(40),YDIF(30),ZDIF(30),FXP(40),FXM(40),     COMMON      4
     2  FYP(30),FYM(30),FZP(30),FZM(30),DT,TIME                         COMMON      5
      COMMON                                                            NOX         2
     1/CINDEX/IDCC,IDFU,IDO2,IDN2,IDH2O,IDCO2,IDH1,IDH2,IDN1,IDNO,IDNO2 NOX         3
     1,IDO,IDOH,IHCPS,ILC,ILH,IMAT,ITER,JJJ,N1,N2,N3,NA,NGLOB,NGLOBP,   NOX         4
     2 NLM,NQ,NSM,NS1,NS2,IDCH                                          4STEP       3
     3/CCHEMI/CPSUM,HSUM,FQ,PPLN,RGAS,RGASIN,SMINV,TKINV,TLN,LNRG       NOX         5
     4/CPARAM/ASUB(30,3),ENV,ER,HSUBO,NDEBUG,NS,PA,QQ,Q1,Q2,Q3,Q4,RHOPP, NOX        .
     4 SM,SMW(30),SMO,S1(30),S2(30),TK,LADIAB,LDEBUG,LEQUIL,LREACT,     NOX         8
     4 LENER,EORIJ,LCONVG                                               NOX         9
      DOUBLE PRECISION CPSUM,ENV,ER,FQ,HSUBO,HSUM,PA,PPLN,QQ,Q1,Q2,Q3,  NOX        10
     1 Q4,RGAS,RGASIN,RHOPP,SM,SMINV,SMW,S1,S2,TK,TKINV,TLN,SMO         NOX        11
     2,FUT,FST                                                          4STEP       4
      COMMON/STEP4/PEXP1,PEXP2,PEXP3,PEXP4,ER1,ER2,ER3,ER4,CEBU1,CEBU2, 4STEP       5
     1 CEBU3,CEBU4,AEXP1,AEXP2,AEXP3,AEXP4,BEXP1,BEXP2,BEXP3,BEXP4,     4STEP       6
     2 CEXP1,CEXP2,CEXP3,CEXP4,FUT,FST                                  4STEP       7
      LOGICAL LADIAB,LCONVG,LDEBUG,LEQUIL,LNRG,LREACT,LENER             NOX        12
      COMMON/INT/L,M,N,LCV,MCV,NCV,LP1,MP1,NP1,MI,MJ,MK,MINJ,MINJNK,NV,  COMMON      6
     1 NNV,NGOTO,K,ISTR,JSTR,KSTR,NVM(35),KM(30),JM(30),ISTEP,          4STEP       8
     2 ISOLVE(32),IPRINT(33),TITLE(10,33),IXY,ISWP,JSWP,RELAX(35),NP,   4STEP       9
     3  NRHO,NGAM,IWLI(30,5),IWLO(30,5),JWLO(40,5),JWLI(  ,5),IWEI,     COMMON      9
     4  IWEO,MM1,JWII,JWIO,JWOI,JWOO,IDW,JKIN(30,30),IKIN(40,30)        COMMON     10
      COMMON/INDEX/IPAR,LPREF,LSTUN,INCOMP,ITRAO,NVRX,NVRY,NVRZ,JPLANE  COMMON     11
     1,PLANM1,LVK,LVO,LVFUOX,LVFU,LVCO,LVH,LVRX,LVRY,LVRZ,NVF(32),      4STEP      10
     2  IJUMP,IRES,TITLE2(20),IMAX,JMAX,KMAX,NVCO,FUNCO,NVH2O,NVCO2,    COMMON     13
     3 NVN2,NVCH,NVH2                                                   4STEP      11
      COMMON/CNOX/LVH1,LVH2,LVN1,LVNO,LVNO2,LVO,LVOH,LVH2O,LVN2,LVO2,    NOX        16
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     1 LVCO2,LVFU1,LVCO1,NNOX,INOX,ITNOX,SNOX,TNOX                          NOX       17
      COMMON/THERM/NVH,NVFU,NVOX,NVPROX,NVTE,MODEN,IOK,FSTOIC,HFU,CP,       COMMON    15
     1  GASCON,PHOCON,UNICON,PRESS,NVFAV,TCYLW,TINLW,TLIP,ACOEF(4),         COMMON    16
     2  T4,DFAC,WFU,WCO2,WCO,WOX,WH2O,WH2,HYY,CXX,RATIO1,RATIO2,            COMMON    17
     3  RATIO3,RATIO4,HCO,TAN,ITWALL                                        COMMON    18
      COMMON/CTDMA/NEND,ICTDMA(92)                                         4STEP     12
      COMMON/MIS/AMU,DEN,SMAX,SSUM,LASTEP,HTCEXT,CFR,EMISW,EMISIN,         CONGEN     2
     1  EMISP,TOUT,RTCO,ENI,RADIN,RADSUR,FMA,FK,SQFK,                       CONGEN     3
     2  FWFU,FOFU,TFUEL,NFNZ,FLO(40),TEMTM(40),M(40),FUEL(40),FUOX(40) ,    CONGEN     4
     2 UIN(40),TIN(40),FUELS(40),SEKIT,IGAM1(29),IGAM2(29)                  4STEP     13
      COMMON/TURB/NVK,NVD,C1,C2,CD,AK,DUIDXJ(3,3),AKFAC,ALFAC,             CONGEN     6
     1 MODEL,PR(32),PREF(32),PJAV(32),F                                    4STEP     14
      COMMON/RAD/NVE,SIGMA,ABSOR,SCATR                                     CONGEN     8
      COMMON/REACT/ARCON1,PREXP1,CR1,ARCON2,PREXP2,CR2,MODER               CONGEN     9
      COMMON/DROPL/EVAP(192),NTP4,NFNZ,XO(3),YO(3),ZO(3),ALFA(3),          CONGEN    10
     1  BETA(3),DELTA(3),THETA1(3),THETA2(3),NSL(3),WFF(3),SMD(3),          CONGEN    11
     2  VFUEL(3),RFUEL(3),EVSU(64),HEVAP                                    CONGEN    12
      COMMON/INJEC/FLOWIN,IUINJ(20),JUINJ(20),UINJ(20),WUINJ(20),          CONGEN    13
     1  AUINJ(20),TUINJ(20),IVINJ(20),JVINJ(20),RVINJ(20),VINJ(20),         CONGEN    14
     2  EVINJ(20),DVINJ(20),AVINJ(20),TVINJ(20),NUINJ,NVINJ,JSW1,JSW2,      CONGEN    15
     3  USW,VSW,AFSW,FSW,TSW,WSW,SWNO,RHOSW                                 CONGEN    16
      COMMON/CSOOT/NVN,NVS1,NVS2,ISOOT,SSOOT,NSOOT,AO,ARCONN,AAA,BBB,FMG   SOOT       8
     1,GO,MPART,DPART(2),FRACP(2),RHOP,ARCONS,PREXPS,ALPHA,AAS,BBS,DHR     SOOT       9
     2,LVN,LVS1,LVS2,CINCP,TINCP,FUTOT                                     SOOT      10
      COMMON/CRAD/IRAD,SRAD                                                SOOT      11
      COMMON/CFOUR/PREXP3,ARCON3,CR3,PREXP4,ARCON4,CR4,AA1,BB1,CC1,        4STEP     15
     1 AA2,BB2,CC2,AA3,BB3,CC3,AA4,BB4,CC4,RATIO5,RATIO6,RATIO7,           4STEP     16
     2 RATIO8,RATIO9,RATO10,RATO11,RATO12,WCH,WH2,WC2H4,LVCH,LVCH1,LVH21   4STEP     17
      DIMENSION VFCX(30),VECY(30),VECZ(30),DSMD(5),XM(40),YM(30),ZM(30)    SP        12
      DIMENSION PO(4),EE(4),FRACT(7),MW(7),MWCOND(4),ACOND(4),BCOND(4)     SP        13
      DIMENSION EVAPU(192),EVAPV(192),EVAPW(192),RVECX(30),RVECY(30),      NASAX     30
     1 RVECZ(30)                                                           NASAX     31
      REAL MW,MWCOND,MWT                                                   SP        15
C +-+-+-+-+-+-+-+-+-+-+-+-+  BEWARE OF EQUIVALENCE STATEMENTS  +-+-+-+-+-+-+-+-+-+-+ SP  16
      EQUIVALENCE (EVAPU(1),AXMK(1)),(EVAPV(1),AYMK(1))                    SP        17
      EQUIVALENCE (EVAPW(1),AZMK(1))                                       SP        18
C +-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+ SP  19
      DATA DSMD/.6,.9,1.2,1.5,2.1/                                         SP        20
      DATA PO,EE/-114.,41.574,96.534,146.57,41.026,30.857,27.340,23.997/   SP        21
      DATA FRACT,MW/0.,.1,.3,.5,.7,.9,1.,93.26,114.6,126.61,138.16         SP        22
     1              ,150.59,173.21,204.76/                                 SP        23
      DATA ACOND,BCOND,MWCOND/-6.362E-3,-6.358E-3,-6.284E-3,-6.01E-3       SP        24
     1,5.36E-5,4.91E-5,4.66E-5,4.23E-5,50.,100.,150.,300./                 SP        25
      DATA NG,RNG,PI,PI2/9,5.,3.14159,6.28318/                             SP        26
C ***************************************************************        SP        27
C ------------SOME PRELIMINARIES                                          SP        28
      IF (NFNZ.LE.0) RETURN                                                SP        29
      SC3=.9283                                                            SP        30
      PR3=.9283                                                            SP        31
      DLIM=.1                                                              SP        32
      ULIM=.1                                                              SP        33
      TF=2300.                                                             SP        34
      HEVAP=30670.6*(1092.88-1.8*TFUEL)**.39                               SP        35
      HFUEL=4.5E+7                                                         SP        36
      ROFO=1000.*(.775+.208-.00072*TFUEL)                                  SP        37
      ZSMALL=(Z(NP1)-Z(1))/FLOAT(NP1)/100.                                 SP        38
      DO 7 K=2,N                                                           SP        39
      DO 7 J=2,M                                                           SP        40
      DO 7 I=2,L                                                           SP        41
      LPC=I-1+(J-2)*(NI-2)+(K-2)*(NI-2)*(NJ-2)                             SP        42
      EVAPU(LPC)=0.                                                        SP        43
      EVAPV(LPC)=0.                                                        SP        44
      EVAPW(LPC)=0.                                                        SP        45
    7 EVAP(LPC)=0.                                                         SP        46
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      XM(1)=X(1)                                                        SP       47
      DO 115 I=2,L                                                      SP       48
  115 XM(I)=XM(I-1)+XS(I)                                               SP       49
      XM(LP1)=XM(L)                                                     SP       50
      YM(1)=Y(1)                                                        SP       51
      DO 17 J=2,M                                                       SP       52
   17 YM(J)=YM(J-1)+YS(J)                                               SP       53
      YM(MP1)=YM(M)                                                     SP       54
      ZM(1)=Z(1)                                                        SP       55
      DO 19 K=2,N                                                       SP       56
   19 ZM(K)=ZM(K-1)+ZS(K)                                               SP       57
      ZM(NP1)=ZM(N)                                                     SP       58
C ***************************************************************      SP       59
C ---------LOOP OVER FUEL NOZZLES                                       SP       60
      DO 2000 NN=1,NFN7                                                 SP       61
      AFF=0.                                                            SP       62
      NSL2=NSL(NN)                                                      SP       63
      RNSL=NSL2                                                         SP       64
      WFI=WFF(NN)/RNSL                                                  SP       65
C ---------CALCULATE UNIT VECTORS OF SPRAY LINES                        SP       66
      SINA=SIN(ALFA(NN)/2.)                                             SP       67
      SINB=SIN(BETA(NN))                                                SP       68
      SIND=SIN(DELTA(NN))                                               SP       69
      COSA=COS(ALFA(NN)/2.)                                             SP       70
      COSB=COS(BETA(NN))                                                SP       71
      COSD=COS(DELTA(NN))                                               SP       72
      DTHETA=THETA2(NN)-THETA1(NN)                                      SP       73
      IF (DTHETA.LT.0.0) DTHETA=DTHETA+PT2                              SP       74
      DANG=DTHETA/(RNSL-1.)                                             SP       75
      IF (DTHETA.GT.0.98*PT2) DANG=DTHETA/RNSL                          SP       76
      THETA=THETA1(NN)                                                  SP       77
      DO 10 IL=1,NSL2                                                   SP       78
      SINT=SIN(THETA)                                                   SP       79
      COST=COS(THETA)                                                   SP       80
      THETA=THETA+DANG                                                  SP       81
      IF (THETA.GT.PT2) THETA=THETA-PT2                                 SP       82
      VECX(IL)=-SINA*SINT*COSB-COSA*SINB                                SP       83
      VECY(IL)=SINA*COST*COSD+SINA*SINT*SINB*SIND-COSA*COSB*SIND        SP       84
      VECZ(IL)=SINA*COST*SIND-SINA*SINT*SINB*COSD+COSA*COSB*COSD        SP       85
      RVECX(IL)=-SINT*COSB                                              SP       86
      RVECY(IL)=COST*COSD+SINT*SINB*SIND                                SP       87
      RVECZ(IL)=COST*SIND-SINT*SINB*COSD                                SP       88
   10 CONTINUE                                                          SP       89
C***************************************************************       SP       90
C------START CALCULATIONS FOR EVAPORATION RATES-----------------------  SP       91
      DO 1000 IL=1,NSL2                                                 SP       92
      DO 1000 IG=1,NG                                                   SP       93
      UF=VECX(IL)*VFUEL(NN)                                             SP       94
      VF=VECY(IL)*VFUEL(NN)                                             SP       95
      WF=VECZ(IL)*VFUEL(NN)                                             SP       96
      DIA=SMD(NN)*1.E-6*DSMD(IG)                                        SP       97
      TFU=TFUEL                                                         SP       98
      ITYPE=1                                                           SP       99
      DIA0=DIA                                                          SP      100
      CON2=0.                                                           SP      101
      IGPNT=-10                                                         SP      102
      IF (ISTEP.NE.IGPNT) GO TO 7746                                    SP      103
      WRITE (6,7747)                                                    SP      104
 7747 FORMAT (/10X,'UF',10X,'VF',10X,'WF',9X,'UST',9X,'VST',9X,'WST',   SP      105
     1 7X,'FEVAP',10X,'XF',10X,'YF',10X,'ZF')                           SP      106
 7746 CONTINUE                                                          SP      107
      FEVAP=0.                                                          SP      108
      DO 11 I=1,LP1                                                     SP      109
      IL0C=I                                                            SP      110
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      IF (XO(NN).GT.XM(I)) GO TO 11                                    SP      111
      GO TO 12                                                         SP      112
   11 CONTINUE                                                         SP      113
   12 DO 13 J=1,NP1                                                    SP      114
      JLOC=J                                                           SP      115
      IF (YO(NN).GT.YM(J)) GO TO 13                                    SP      116
      GO TO 14                                                         SP      117
   13 CONTINUE                                                         SP      118
   14 DO 15 K=1,NP1                                                    SP      119
      KLOC=K                                                           SP      120
      IF (ZO(NN).GT.ZM(K)) GO TO 15                                    SP      121
      GO TO 16                                                         SP      122
   15 CONTINUE                                                         SP      123
   16 XF=XO(NN)+RFUEL(NN)*RVECX(IL)                                    SP      124
      YF=YO(NN)+RFUEL(NN)*RVECY(IL)                                    SP      125
      ZF=ZO(NN)+RFUEL(NN)*RVECZ(IL)/(R(1)+PLAXM1*YF)                   SP      126
C-----LOCATION OF THE DROPLET-----------                               SP      127
  110 CONTINUE                                                         SP      128
      ILOLD=ILOC                                                       SP      129
      JOLD=JLOC                                                        SP      130
      KOLD=KLOC                                                        SP      131
C ----X DROPLET LOCATION                                               SP      132
      IF (XF.GE.XM(ILOC-1).AND.XF.LT.XM(ILOC)) GO TO 27                SP      133
      DO 22 I=1,LP1                                                    SP      134
      ILOC=I                                                           SP      135
      IF (XF.GT.XM(I)) GO TO 22                                        SP      136
      GO TO 27                                                         SP      137
   22 CONTINUE                                                         SP      138
C ----Y DROPLET LOCATION                                               SP      139
   27 IF (YF.GE.YM(JLOC-1).AND.YF.LT.YM(JLOC)) GO TO 23                SP      140
      DO 24 J=1,NP1                                                    SP      141
      JLOC=J                                                           SP      142
      IF (YF.GT.YM(J)) GO TO 24                                        SP      143
      GO TO 23                                                         SP      144
   24 CONTINUE                                                         SP      145
C ----Z DROPLET LOCATION                                               SP      146
   23 IF (ZF.GE.ZM(KLOC-1).AND.ZF.LT.ZM(KLOC)) GO TO 63                SP      147
      DO 26 K=1,NP1                                                    SP      148
      KLOC=K                                                           SP      149
      IF (ZF.GT.ZM(K)) GO TO 26                                        SP      150
      GO TO 48                                                         SP      151
   26 CONTINUE                                                         SP      152
   48 IF (KLOC.GT.1) GO TO 28                                          SP      153
      KLOC=N                                                           SP      154
      ZF=Z(NP1)-ZSMALL                                                 SP      155
   28 IF (KLOC.LT.NP1) GO TO 63                                        SP      156
      KLOC=2                                                           SP      157
      ZF=Z(1)+ZSMALL                                                   SP      158
C ----DROPLET NEAR A WALL                                              SP      159
   63 INDX=0                                                           SP      160
      IF (ILOC.GE.IWLI(JLOC,4)) GO TO 43                               SP      161
      ILOC=ILOLD                                                       SP      162
      XF=AMAX1(XF,XM(ILOC-1)+DIA/2.)                                   SP      163
      XF=AMIN1(XF,XM(ILOC)-DIA/2.)                                     SP      164
      INDX=1                                                           SP      165
   43 IF (ILOC.LE.IWLO(JLOC,4)) GO TO 47                               SP      166
      IF (JLOC.GT.JWOI.AND.JLOC.LT.JWOO) GO TO 1000                    SP      167
      ILOC=ICLD                                                        SP      168
      XF=AMAX1(XF,XM(ILOC-1)+DIA/2.)                                   SP      169
      XF=AMIN1(XF,XM(ILOC)-DIA/2.)                                     SP      170
      INDX=2                                                           SP      171
   47 IF (JLOC.GT.JWLI(ILOC,4)) GO TO 44                               SP      172
      IF (IOW.EQ.0) GO TO 50                                           SP      173
      JLOC=JOLD                                                        SP      174
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      YF=AMAX1(YF,YM(JLOC-1)+DIA/2.)                                    SP        175
      YF=AMIN1(YF,YM(JLOC)-DIA/2.)                                      SP        176
      INDX=3                                                            SP        177
   44 IF (JLOC.LT.JWLO(ILOC,4)) GO TO 41                                SP        178
      JLOC=JOLD                                                         SP        179
      YF=AMAX1(YF,YM(JLOC-1)+DIA/2.)                                    SP        180
      YF=AMIN1(YF,YM(JLOC)-DIA/2.)                                      SP        181
      INDX=4                                                            SP        182
C ----CHECK FOR SLOTS                                                   SP        183
   41 IF (NUINJ.LE.0) GO TO 45                                          SP        184
      DO 149 II=1,NUINJ                                                 SP        185
      IU=IUINJ(II)-1                                                    SP        186
      JU=JUINJ(II)                                                      SP        187
      IF (ILOC.EQ.IU.AND.JLOC.EQ.JU) GO TO 50                           SP        188
  149 CONTINUE                                                          SP        189
   45 CONTINUE                                                          SP        190
      GO TO 60                                                          SP        191
C --------DROPLET HAS HIT SOLID BOUNDRY                                 SP        192
   50 ILOC=ICLD                                                         SP        193
      JLOC=JOLD                                                         SP        194
      KLOC=KOLD                                                         SP        195
      DEVAP=1.-FEVAP                                                    SP        196
      UF=0.                                                             SP        197
      VF=0.                                                             SP        198
      WF=0.                                                             SP        199
      FX=0.                                                             SP        200
      FY=0.                                                             SP        201
      FZ=0.                                                             SP        202
      GO TO 249                                                         SP        203
C --------NO BOUNDRIES HAVE BEEN HIT                                    SP        204
   60 CONTINUE                                                          SP        205
      LP=KM(KLOC)+JM(JLOC)+ILOC                                         SP        206
      LYP=LP+1                                                          SP        207
      LYP=LP+NI                                                         SP        208
      LZP=LP+NINJ                                                       SP        209
      LPTE=LP+NVM(NVTE)                                                 SP        210
      LPFUDX=LP+NVM(NVFUDX)                                             SP        211
C -------- CAREFUL HERE                                                SP        212
      LPFU=LP+NVM(NVFU+3)                                               SP        213
      LPCO=LP+NVM(NVCO+1)                                               SP        214
      LPCH=LP+NVM(NVCH)                                                 4STEP     326
      LPH2=LP+NVM(NVH2)                                                 4STEP     327
C ----FREESTREAM PROPERTIES                                             SP        215
      ROST=RHO(LP)                                                      SP        216
      TST=F(LPTE)                                                       SP        217
      UST=FXP(ILOC)*U(LP)+FXM(ILOC)*U(LXP)                              SP        218
      VST=FYP(JLOC)*V(LP)+FYM(JLOC)*V(LYP)                              SP        219
      WST=FZP(KLOC)*W(LP)+FZM(KLOC)*W(LZP)                              SP        220
      IB=IWLI(JLOC,4)                                                   SP        221
      IF (XF.GE.X(IB)) GO TO 51                                         SP        222
      IF (JKIN(JLOC,KLOC).EQ.1) GO TO 51                                SP        223
      FAC=((XF-XM(IB-1))/(X(IB)-XM(IB-1)))**.14286                      SP        224
      UST=0.                                                            SP        225
      VST=VST*FAC                                                       SP        226
      WST=WST*FAC                                                       SP        227
      IF (INDX.NE.1) GO TO 51                                           SP        228
      UF=UST                                                            SP        229
      VF=VST                                                            SP        230
      WF=WST                                                            SP        231
   51 IB=IWLO(JLOC,4)                                                   SP        232
      IF (XF.LE.X(IB)) GO TO 56                                         SP        233
      IF (JLOC.GT.JWOI.AND.JLOC.LT.JWOO) GO TO 56                       SP        234
      FAC=((XM(IB)-XF)/(XM(IB)-X(IB)))**.14286                          SP        235
      UST=0.                                                            SP        236
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      VST=VST*FAC                                                       SP      237
      WST=WST*FAC                                                       SP      238
      IF (INOX.NE.2) GO TO 56                                           SP      239
      UF=UST                                                            SP      240
      VF=VST                                                            SP      241
      WF=WST                                                            SP      242
   56 JB=JWLI(ILOC,4)                                                   SP      243
      IF (YF.GE.Y(JB+1)) GO TO 53                                       SP      244
      IF (IKIN(ILOC,KLOC).EQ.1.OR.IKIN(ILOC,KLOC).EQ.3) GO TO 53        SP      245
      FAC=((YF-YM(JB))/(Y(JB+1)-YM(JB)))**.14286                        SP      246
      UST=UST*FAC                                                       SP      247
      VST=0.                                                            SP      248
      WST=WST*FAC                                                       SP      249
      IF (INOX.NE.3) GO TO 53                                           SP      250
      UF=UST                                                            SP      251
      VF=VST                                                            SP      252
      WF=WST                                                            SP      253
   53 JB=JWLO(ILOC,4)                                                   SP      254
      IF (YF.LE.Y(JB-1)) GO TO 5'                                       SP      255
      IF (IKIN(ILOC,KLOC).EQ.2.OR.IKIN(ILOC,JLOC).EQ.3) GO TO 54        SP      256
      FAC=((YM(JB-1)-YF)/(YM(JB-1)-Y(JB-1)))**.14286                    SP      257
      UST=UST*FAC                                                       SP      258
      VST=0.                                                            SP      259
      WST=WST*FAC                                                       SP      260
      IF (INOX.NE.4) GO TO 54                                           SP      261
      UF=UST                                                            SP      262
      VF=VST                                                            SP      263
      WF=WST                                                            SP      264
   54 CONTINUE                                                          SP      265
      IF(ABS(UF).LT.1.E-30.AND.ABS(VF).LT.1.E-30.AND.ABS(UST).LT.1.E-30. NASAX    32
     1 AND.ABS(VST).LT.1.E-30)GO TO 50                                  NASAX    33
      FLPOX=RATIO1*F(LPFU)+RATIO3*F(LPCO)+RATIO2-(RATIO2+RATIO1)*       SP      266
     1 F(LPFUOX)+RATIO5*F(LPCH)+RATIO6*F(LPH2)                          4STEP   328
      FLPOX=AMAX1(FLPOX,0.)                                             SP      268
      IF (ISTEP.NE.IGPNT) GO TO 7744                                    SP      269
      WRITE (6,7745) UF,VF,WF,UST,VST,WST,FEVAP,XF,YF,ZF                SP      270
 7745 FORMAT (10E12.4)                                                  SP      271
 7744 CONTINUE                                                          SP      272
C ----BOILING TEMPERATURE OF FUEL-------------------------------------- SP      273
      POT=PO(4)                                                         SP      274
      ET=EE(4)                                                          SP      275
      IF(FEVAP.GE.0.5) GO TO 200                                        SP      276
      POT=TAB(FEVAP,FRACT,PO,4)                                         SP      277
      ET=TAB(FEVAP,FRACT,EE,4)                                          SP      278
  200 TB=ET*ALOG(PRESS)+POT                                             SP      279
      T1=(TB+TF)/2.                                                     SP      280
      TFU=AMIN1(TFU,T8)                                                 SP      281
C-----DENSITY OF LIQUID FUEL AT TB                                      SP      282
      ROF=1.076/(1.+(1.076/.775-1.)*(1.-.67*FEVAP))                     SP      283
      ROF=1000.*(ROF+.208-.00072*TFU)                                   SP      284
C-----MOLECULAR WEIGHT OF FUEL VAPORS                                   SP      285
      MWT=TAB(FEVAP,FRACT,MW,7)                                         SP      286
      AT=TAB(MWT,MWCOND,ACOND,4)                                        SP      287
  300 BT=TAB(MWT,MWCOND,BCOND,4)                                        SP      288
C-----THERMAL CONDUCTIVITY AND SPECIFIC HEAT OF FUEL VAPORS             SP      289
      COND1=1.7290*(AT+BT*T1)                                           SP      290
      IHCPS=1                                                           NOX     195
      NS1=IDFU                                                          NOX     196
      NS2=IDFU                                                          NOX     197
      TK=T1                                                             NOX     198
      TKINV=1.000/TK                                                    NOX     199
      S2(IDFU)=1.000/SMW(IDFU)                                          NOX     200
      CALL HCPS                                                         NOX     201
      CP1=CPSUM*UNICON                                                  NOX     202
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  400 COND1=0.4*COND1+0.6*.064*SQRT(T1/1111.)                          SP        292
C ----RELATIVE VEL. REYNOLDS NO.,DRAG COEF AND FORCE COMPONENTS        SP        293
      VR=SQRT((UF-UST)**2+(VF-VST)**2+(WF-WST)**2)                     SP        294
      VISCO=4.464E-5*SQRT(TST/1111.)                                   SP        295
      REI=ROST*VR*DIA/VISCO                                            SP        296
      SREI=SQRT(REI)                                                   SP        297
      COS=2.0                                                          SP        298
      IF (REI.GT.22.16.AND.REI.LE.80.) COS=27./REI**.84                SP        299
      IF (REI.GT.80..AND.REI.LT.10000.) COS=.271*REI**.217             SP        300
      CD1=AMAX1(COS/2.,COS/(1.+BEE))                                   SP        301
      CONS=CD1*3.14159/4.*DIA**2/2.*ROST                               SP        302
      DM=PI*DIA**3*ROF/6.                                              SP        303
      FX=CONS*VR*(UST-UF)                                              NASAX      34
      FY=CONS*VR*(VST-VF)+PLAXM1*DM*WF*WF/R(JLOC)                      NASAX      35
      FZ=CONS*VR*(WST-WF)-PLAXM1*DM*VF*WF/R(JLOC)                      NASAX      36
      VFU=SQRT(UF**2+VF**2+WF**2)                                      SP        307
      FAC=AMAX1(1.0,25./(VR*VR+1.E-20))                                SP        308
      DTI1=ULIM*VFU*DM*FAC/(ABS(FX)+1.E-30)                            SP        309
      DTI2=ULIM*VFU*DM*FAC/(ABS(FY)+1.E-30)                            SP        310
      DTI3=ULIM*VFU*DM*FAC/(ABS(FZ)+1.E-30)                            SP        311
      DTI4=DLIM/(CON2+1.E-30)                                          SP        312
      DTI5=XS(ILOC)/(ABS(UF)+1.E-20)                                   SP        313
      DTI6=YS(JLOC)/(ABS(VF)+1.E-20)                                   SP        314
      DTI7=R(JLOC)*ZS(KLOC)/(ABS(WF)+1.E-20)                           SP        315
      DTI=AMIN1(DTI1,DTI2,DTI3,DTI4,DTI5,DTI6,DTI7)                    SP        316
      CONS=DM/DTI                                                      SP        317
C-----VELOCITY AND LOCATION OF THE DROPLET                             SP        318
      UFO=UF                                                           SP        319
      VFO=VF                                                           SP        320
      WFO=WF                                                           SP        321
      UF=UF+FX/CONS                                                    SP        322
      VF=VF+FY/CONS                                                    SP        323
      WF=WF+FZ/CONS                                                    SP        324
      IF (UFO.GT.UST) UF=AMAX1(UF,UST-.001)                            SP        325
      IF (UFO.LT.UST) UF=AMIN1(UF,UST+.001)                            SP        326
      IF (VFO.GT.VST) VF=AMAX1(VF,VST-.001)                            SP        327
      IF (VFO.LT.VST) VF=AMIN1(VF,VST+.001)                            SP        328
      IF (WFO.GT.WST) WF=AMAX1(WF,WST-.001)                            SP        329
      IF (WFO.LT.WST) WF=AMIN1(WF,WST+.001)                            SP        330
      DX=.5*(UF+UFO)*DTI                                               SP        331
      DY=.5*(VF+VFO)*DTI                                               SP        332
      DZ=.5*(WF+WFO)*DTI                                               SP        333
      XF=XF+DX                                                         SP        334
      YF=YF+DY                                                         SP        335
      ZF=ZF+DZ/R(JLOC)                                                 SP        336
      IF (TFU.GE.TB) ITYPE=2                                           SP        337
      GO TO (188,199), ITYPE                                           SP        338
C----------   HEATING DROPLET  ---------------------------------------- SP        339
C ----HEAT TRANSFER                                                    SP        340
  188 HT=COND1*(2.+.6*PR3*SREI)/DIA                                    SP        341
      AS=PI*DIA*DIA                                                    SP        342
      QDOT=AS*HT*(TST-TFU)                                             SP        343
      CPLF=8440.*4.1372*TFU                                            SP        344
      DTF=DTI*QDOT/DM/CPLF                                             SP        345
      TFU=TFU+DTF                                                      SP        346
      GO TO 110                                                        SP        347
C ----------   BOILING DROPLET  ---------------------------------      SP        348
C-----MASS TRANSFER NUMBER                                             SP        349
  198 IF (F(LFUCK)-FSTOIC) 210,209,201                                 SP        350
  201 BEE=AMAX1(CP1*(TST-TB)/HEVAP,0.)                                 SP        351
      GO TO 219                                                        SP        352
  209 BEE=FLPOX/RATIO1                                                 SP        353
      GO TO 219                                                        SP        354
  210 BEE=(FLPOX*HFUEL/RATIO1+AMAX1(CP1*(TST-TB),0.))/HEVAP            SP        355
210
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  210 RATE=8./ROF*CON01/CP1*ALOG(1.+BEE)*(1.+0.276*SREI*SC8)                SP      356
C-----FRACTION EVAPORATED                                                   SP      357
      CON2=1.5/ROFD/DIA0**3*ROF*DIA*RATE                                    SP      358
      DEVAP=CON2*DTI                                                        SP      359
  240 FEVAP=FEVAP+DEVAP                                                     SP      360
      IF (FEVAP.LT.1.0) GO TO 250                                           SP      361
      DEVAP=DEVAP-FEVAP+1.                                                  SP      362
      FEVAP=1.                                                              SP      363
C ----NEW DROPLET DIAMETER                                                  SP      364
  250 ARG=DIA*DIA-RATE*DTI                                                  SP      365
      IF (ARG.GT.0.0) GO TO 262                                             SP      366
      DEVAP=DEVAP+1.-FEVAP                                                  SP      367
      FEVAP=1.0                                                             SP      368
      GO TO 292                                                             SP      369
  262 DIA=SQRT(ARG)                                                         SP      370
C ---------- FUEL EVAPORATION FLOW RATE  ----------                        SP      371
  292 AMT=DEVAP*WFI/RNG                                                     SP      372
      LPC=ILOC-1+(JLOC-2)*(NI-2)+(KLOC-2)*(NI-2)*(NJ-2)                     SP      373
      EVAP(LPC)=EVAP(LPC)+AMT                                               SP      374
      EVAPU(LPC)=EVAPU(LPC)+AMT*UF                                          SP      375
      EVAPV(LPC)=EVAPV(LPC)+AMT*VF                                          SP      376
      EVAPW(LPC)=EVAPW(LPC)+AMT*WF                                          SP      377
  900 IF (FEVAP.LT.0.99) GO TO 110                                          SP      378
 1000 CONTINUE                                                              SP      379
 2000 CONTINUE                                                              SP      380
C ***************************************************************************SP      381
C ------ STORE MOMENTUM DATA ON TAPE4                                       SP      382
      REWIND NTP4                                                           SP      383
      DO 1100 K=2,N                                                         SP      384
      DO 1110 J=2,M                                                         SP      385
      KJC=(K-2)*(NI-2)*(NJ-2)+(J-2)*(NI-2)                                  SP      386
      DO 1110 I=3,L                                                         SP      387
      LIJ=(J-2)*(NI-2)+(I-1)                                                SP      388
      LPC=KJC+(I-1)                                                         SP      389
      LXMC=LPC-1                                                            SP      390
      EVSU(LIJ)=FXM(I-1)*EVAPU(LXMC)+SXP(I)*EVAPU(LPC)                      SP      391
      IF (I.EQ.3) EVSU(LIJ)=EVSU(LIJ)+FXP(2)*EVAPU(LXMC)                    SP      392
      IF (I.EQ.L) EVSU(LIJ)=EVSU(LIJ)+FXM(L)*EVAPU(LPC)                     SP      393
 1110 CONTINUE                                                              SP      394
      WRITE (NTP4) EVSU                                                     SP      395
 1100 CONTINUE                                                              SP      396
      DO 1200 K=2,N                                                         SP      397
      DO 1210 J=3,M                                                         SP      398
      KJC=(K-2)*(NI-2)*(NJ-2)+(J-2)*(NI-2)                                  SP      399
      DO 1210 I=2,L                                                         SP      400
      LIJ=(J-2)*(NI-2)+(I-1)                                                SP      401
      LPC=KJC+(I-1)                                                         SP      402
      LYMC=LPC-(NI-2)                                                       SP      403
      EVSU(LIJ)=FYM(J-1)*EVAPV(LYMC)+FYP(J)*EVAPV(LPC)                      SP      404
      IF (J.EQ.3) EVSU(LIJ)=EVSU(LIJ)+FYP(2)*EVAP(LYMC)                     SP      405
      IF (J.EQ.M) EVSU(LIJ)=EVSU(LIJ)+FYM(M)*EVAPV(LPC)                     SP      406
 1210 CONTINUE                                                              SP      407
      WRITE (NTP4) EVSU                                                     SP      408
 1200 CONTINUE                                                              SP      409
      DO 1300 K=3,NP1                                                       SP      410
      DO 1310 J=2,M                                                         SP      411
      KJC=(K-2)*(NI-2)*(NJ-2)+(J-2)*(NI-2)                                  SP      412
      DO 1310 I=2,L                                                         SP      413
      LIJ=(J-2)*(NI-2)+(I-1)                                                SP      414
      LPC=KJC+(I-1)                                                         SP      415
      LZMC=LPC-(NI-2)*(NJ-2)                                                SP      416
      EVSU(LIJ)=FZM(K-1)*EVAPW(LZMC)                                        SP      417
      IF (K.EQ.NP1) GO TO 1309                                              SP      418
      EVSU(LIJ)=EVSU(LIJ)+FZP(K)*EVAPW(LPC)                                 SP      419
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      GO TO 1310                                                        SP        420
 1309 EVSU(LIJ)=EVSU(LIJ)+FZP(2)*EVAPM(LIJ)                             SP        421
 1310 CONTINUE                                                          SP        422
      WRITE (NTP4) EVSU                                                 SP        423
 1300 CONTINUE                                                          SP        424
      RETURN                                                            SP        425
      END                                                               SP        426
      FUNCTION TAB (X,XX,YY,NTAB)                                       SP        427
      DIMENSION XX(1),YY(1)                                             SP        428
      IF (NTAB.GT.0) GO TO 5                                            SP        429
      TAB=0.0                                                           SP        430
      RETURN                                                            SP        431
    5 F=1.                                                              SP        432
      IF (XX(1).GT.XX(2)) F=-F                                          SP        433
      DO 10 J=1,NTAB                                                    SP        434
      I=J                                                               SP        435
      IF (F*(XX(I)-X)) 10,40,20                                         SP        436
   10 CONTINUE                                                          SP        437
   20 IF (I.NE.1) GO TO 30                                              SP        438
      I=2                                                               SP        439
   30 J=I-1                                                             SP        440
      DEL=XX(I)-XX(J)                                                   SP        441
      IF (DEL.EQ.0.0) GO TO 50                                          SP        442
      TAB=(YY(I)*(X-XX(J))-YY(J)*(X-XX(I)))/DEL                         SP        443
      RETURN                                                            SP        444
   40 TAB=YY(I)                                                         SP        445
      RETURN                                                            SP        446
   50 WRITE (6,60) X,I,J                                                SP        447
   60 FORMAT (' *** ERROR IN SUBROUTINE TAB ***',E15.4,2I5)             SP        448
      STOP                                                              SP        449
      END                                                               SP        450
      SUBROUTINE STRIDE                                                 ST          2
      COMMON/CEDK/EDK(192)                                              NOX       203
      COMMON F(3500),DU(500),DV(500),DW(500),                           COMFB       2
     1 ANUC(500),SOOT1(500),SOOT2(500),FCH(500),FH2(500),FS(500,14),    4STEP      18
     1 RHO(500),VISC(500),ABSR(500),SCTR(500),SU(100),SP(100),          RAD         3
     1 DRHODP(500),                                                     RAD         4
     1  AXP(100),AXM(100),AYP(100),AYM(100),AZP(100),                   COMFB       4
     2  AZM(100),CZ(100),CY(10),CZU(100),CYU(10),                       COMFB       5
     3  CZP(100),CYP(10),DIVG(100),NTP1,NTP2                            COMFB       6
     1,AXMK(192),AXPK(192),AYMK(192),AYPK(192),AZMK(192),AZPK(192),     CTDMA       3
     2 SUK(192),SPK(192)                                                CTDMA       4
      DIMENSION U(500),V(500),W(500),PP(500),P(500),TEMP(500)           COMFB       7
      DIMENSION GAM(500)                                                COMFB       8
      EQUIVALENCE (F(1),U(1)),(F(501),V(1)),(F(1001),W(1))              COMFB       9
      EQUIVALENCE (F(1501),PP(1)),(F(2001),P(1)),(F(2501),TEMP(1))      COMFB      10
      EQUIVALENCE (F(3001),GAM(1))                                      COMFB      11
      COMMON/CYL/R(30),RM(30),RMV(30),YSR(30),YSVR(30),IPLAN            COMMON      2
      COMMON/GRID/X(40),Y(30),Z(30),XS(40),YS(30),ZS(30),XSU(40),       COMMON      3
     1  YSV(30),ZSW(30),XDIF(40),YDIF(30),ZDIF(30),FXP(40),FXM(40),     COMMON      4
     2  FYP(30),FYM(30),FZP(30),FZM(30),DT,TIME                         COMMON      5
      COMMON                                                            NOX         2
     1/CINDEX/IDCO,IDFU,IDO2,IDN2,IDH2O,IDCO2,IDH1,IDH2,IDN1,IDNO,IDNO2 NOX         3
     1,IDO,IDOH,IMCPS,ILC,ILH,IMAT,ITER,JJJ,N1,N2,N3,NA,NGLOB,NGLOBP,   NOX         4
     2 NLM,NQ,NSM,NS1,NS2,IDCH                                          4STEP       3
     3/CCHEM1/CPSUM,HSUM,FQ,PPLN,RGAS,RGASIN,SMINV,TKINV,TLN,LNRG       NOX         6
     4/CPARAM/ASUR(30,3),EMV,EP,HSUBO,NDEBUG,NS,PA,QQ,Q1,Q2,Q3,Q4,RHOPP, NOX         7
     4 SM,SMW(30),SMO,S1(30),S2(30),TK,LADIAB,LDEBUG,LEQUIL,LREACT,     NOX         8
     4 LENEP,FDKIJ,LCONVG                                               NOX         9
      DOUBLE PRECISION CPSUM,EMV,ER,FQ,HSUBO,HSUM,PA,PPLN,QQ,Q1,Q2,Q3,  NOX        10
     1 Q4,RGAS,RGASIN,RHOPP,SM,SMINV,SMW,S1,S2,TK,TKINV,TLN,SMO         NOX        11
     2,FUT,FST                                                          4STEP       4
      COMMON/STEP4/PEXP1,PEXP2,PEXP3,PEXP4,ER1,ER2,ER3,ER4,CERU1,CERU2, 4STEP       5
     1 CERU3,CERU4,AEXP1,AEXP2,AEXP3,AEXP4,BEXP1,BEXP2,BEXP3,BEXP4,     4STEP       6
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     2 CEXP1,CEXP2,CEXP3,CEXP4,FUT,FST                                  4STEP     7
       LOGICAL LADIAB,LCONVG,LDEBUG,LEQUIL,LNRG,LREACT,LENER            NOX      12
       COMMON/INT/L,M,N,LCV,MCV,NCV,LP1,MP1,NP1,NI,NJ,NK,NINJ,NINJNK,NV, COMMON    6
     1 NNV,NGOTO,K,ISTR,JSTR,KSTR,NVM(35),KM(30),JM(30),ISTEP,          4STEP     8
     2 ISOLVE(32),IPRINT(33),TITLE(10,33),IXY,ISWP,JSWP,RELAX(35),NP,   4STEP     9
     3   NRHO,NGAM,IWLI(30,5),IWLO(30,5),JWLO(40,5),JWLI(40,5),IWEI,    COMMON    9
     4   IWEO,MM1,JWII,JWIO,JWOI,JWOO,IOW,JKIN(30,30),IKIN(40,30)       COMMON   10
       COMMON/INDEX/IPAR,LPREF,ISTUN,INCOMP,ITRAD,NVRX,NVRY,NVRZ,JPLANE COMMON   11
     1,PLANM1,LVK,LVD,LVFUOX,LVFU,LVCO,LVH,LVRX,LVRY,LVRZ,NVF(32),      4STEP    10
     2   TJUMP,IRES,TITLE2(20),IMAX,JMAX,KMAX,NVCO,FUNCO,NVH2O,NVCO2,   COMMON   13
     3 NVN2,NVCH,NVH2                                                   4STEP    11
       COMMON/CNOX/LVH1,LVH2,LVN1,LVNO,LVNO2,LVO,LVOH,LVH2O,LVN2,LVO2,  NOX      16
     1 LVCO2,LVFU1,LVCO1,NNOX,INOX,ITNOX,SNOX,TNOX                      NOX      17
       COMMON/THERM/NVH,NVFU,NVOX,NVFUOX,NVTE,MODEN,IOK,FSTOIC,HFU,CP,  COMMON   15
     1   GASCON,RHOCON,UNICON,PRESS,NVFAV,TCYLW,TINLW,TLIP,ACOEF(4),    COMMON   16
     2   T4,OFAC,WFU,WCO2,WCO,WOX,WH2O,WN2,HYY,CXX,RATIO1,RATIO2,        COMMON   17
     3   RATIO3,RATIO4,HCO,TAN,ITWALL                                   COMMON   18
       COMMON/CTOMA/KEND,ICTOMA(32)                                     4STEP    12
       COMMON/MIS/AMU,DEN,SMAX,SSUM,LASTEP,HTCEXT,CFR,EMISW,EMISIN,     CONGEN    2
     1   EMISP,TOUT,RTCD,EMI,RADIN,RADSUR,FNA,FK,SQFK,                  CONGEN    3
     2   FKFU,FOFU,TFUEL,WFNZ,FLO(40),TEMTM(40),H(40),FUEL(40),FUOX(40) , CONGEN    4
     3 UIN(40),TIN(40),FUELS(40),SEXIT,IGAM1(29),IGAM2(29)              4STEP    13
       COMMON/TURB/NVK,NVD,C1,C2,CD,AK,DUIDXJ(3,3),AKFAC,ALFAC,         CONGEN    6
     1 MODFL,PR(32),PREF(32),PJAY(32),E                                 4STEP    14
       COMMON/RAD/NVE,SIGMA,ABSOR,SCATR                                 CONGEN    8
       COMMON/REACT/ARCON1,PREXP1,CR1,ARCON2,PREXP2,CR2,MODER           CONGEN    9
       COMMON/DROPL/EVAP(192),NTP4,NFNZ,XO(3),YO(3),ZO(3),ALFA(3),      CONGEN   10
     1   BETA(3),DELTA(3),THETA1(3),THETA2(3),NSL(3),WFF(3),SMD(3),      CONGEN   11
     2   VFUEL(3),RFUEL(3),EVSU(64),HEVAP                               CONGEN   12
       COMMON/INJEC/FLOWIN,IUINJ(20),JUINJ(20),UINJ(20),WUINJ(20),      CONGEN   13
     1   AUINJ(20),TUINJ(20),IVINJ(20),JVINJ(20),KVINJ(20),VINJ(20),     CONGEN   14
     2   EVINJ(20),DVINJ(20),AVINJ(20),TVINJ(20),NUINJ,NVINJ,JSW1,JSW2,  CONGEN   15
     3   USW,VSW,AFSW,FSW,TSW,WSW,SWNO,RHOSW                            CONGEN   16
       COMMON/CSOOT/NVN,NVS1,NVS2,ISOOT,SSOOT,NSOOT,AO,ARCONN,AAA,BBB,FMG SOOT     8
     1,GO,MPART,DPART(2),FRACP(2),RHOP,ARCONS,PREXPS,ALPHA,AAS,BBS,DHR   SOOT     9
     2,LVN,LVS1,LVS2,CINCP,TINCP,FUTOT                                  SOOT    10
       COMMON/CRAD/IRAD,SRAD                                            SOOT    11
       COMMON/CFOUR/PREXP3,ARCON3,CR3,PREXP4,ARCON4,CR4,AA1,BB1,CC1,    4STEP    15
     1 AA2,BB2,CC2,AA3,BB3,CC3,AA4,BB4,CC4,RATIO5,RATIO6,RATIO7,        4STEP    16
     2 RATIO8,RATIO9,RATO10,RATO11,RATO12,WCH,WH2,WC2H4,LVCH,LVCH1,LVH21 4STEP    17
       ENTRY STRIDO                                                     ST        5
C-----ENTRY STRIDO IS USED FOR PRELIMINARY CALCULATIONS.                 COMMENT 121
C                                                                       COMMENT 122
       IXY=1                                                            ST        6
       ISWP=1                                                           ST        7
       JSWP=1                                                           ST        8
       TIME=0.                                                          ST        9
       L=LP1-1                                                          ST       10
       M=MP1-1                                                          ST       11
       N=NP1-1                                                          ST       12
       LCV=L-1                                                          ST       13
       MCV=M-1                                                          ST       14
       NCV=N-1                                                          ST       15
       MM1=M-1                                                          ST       16
       NINJ=NI*NJ                                                       ST       17
       NINJNK=NINJ*NK                                                   ST       18
       NVM(1)=0                                                         ST       19
       DO 1 NV=2,NGAM                                                   ST       20
     1 NVM(NV)=NVM(NV-1)+NINJNK                                         ST       21
       KM(1)=0                                                          ST       22
       DO 2 K=2,NP1                                                     ST       23
     2 KM(K)=KM(K-1)+NINJ                                               ST       24
       JM(1)=0                                                          ST       25
       MAX=MAXO(MP1,NP1)                                                ST       26
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```
      DO 3 J=2,MAX                                                      ST        27
      JM(J)=JM(J-1)+NI                                                  ST        28
3     RETURN                                                            ST        29
C  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  ST        30
      ENTRY STRID1                                                      ST        31
C-----ENTRY STRID1 IS USED TO CALCULATE INTER-NODAL DISTANCES,          COMMENT   123
C     CONTROL VOLUME AREAS AND VOLUMES.                                 COMMENT   124
C                                                                       COMMENT   125
C                                                                       COMMENT   126
C-----X-GRID.                                                           ST        32
      DO 101 I=2,LP1                                                    ST        33
101   XDIF(I)=X(I)-X(I-1)                                               ST        34
      DO 111 I=2,L                                                      ST        35
111   XS(I)=0.5*(X(I+1)-X(I-1))                                         ST        36
      XS(2)=XS(2)+0.5*XDIF(2)                                           ST        37
      XS(L)=XS(L)+0.5*XDIF(LP1)                                         ST        38
      DO 121 I=3,L                                                      ST        39
      XSU(I)=XDIF(I)                                                    ST        40
      FXP(I)=XDIF(I)/(2.*XS(I))                                         ST        41
121   FXM(I)=1.-FXP(I)                                                  ST        42
      XSU(3)=XSU(3)+XDIF(2)                                             ST        43
      XSU(L)=XSU(L)+XDIF(LP1)                                           ST        44
      FXP(2)=FXP(3)                                                     ST        45
      FXM(2)=1.-FXP(2)                                                  ST        46
      FXP(L)=FXP(L-1)                                                   ST        47
      FXM(L)=1.-FXP(L)                                                  COMMENT   127
C-----Y-GRID.                                                           ST        48
      DO 102 J=2,MP1                                                    ST        49
102   YDIF(J)= Y(J)- Y(J-1)                                             ST        50
      DO 112 J=2,M                                                      ST        51
112   YS(J)= 0.5*(Y(J+1)-Y(J-1))                                        ST        52
      YS(2)=YS(2)+0.5*YDIF(2)                                           ST        53
      YS(M)=YS(M)+0.5*YDIF(MP1)                                         ST        54
      RM(2)=R(1)                                                        ST        55
      DO 122 J=3,M                                                      ST        56
      RM(J)=.5*(R(J)+R(J-1))                                            ST        57
      RMV(J+1)=R(J)                                                     ST        58
      YSV(J)=YDIF(J)                                                    ST        59
      FYP(J)=YDIF(J)/(2.*YS(J))                                         ST        60
122   FYM(J)=1.-FYP(J)                                                  ST        61
      RM(MP1)=R(MP1)                                                    ST        62
      RMV(3)=R(1)                                                       ST        63
      RMV(MP1)=R(MP1)                                                   ST        64
      YSV(3)=YSV(3)+YDIF(2)                                             ST        65
      YSV(M)=YSV(M)+YDIF(MP1)                                           ST        66
      FYP(2)=FYP(3)                                                     ST        67
      FYM(2)=1.-FYP(2)                                                  ST        68
      FYP(M)=FYP(M-1)                                                   ST        69
      FYM(M)=1.-FYP(M)                                                  ST        70
      DO 132 J=2,M                                                      ST        71
132   YSR(J)=.5*(RM(J+1)+RM(J))*YS(J)                                   ST        72
      DO 142 J=3,M                                                      ST        73
142   YSVR(J)=.5*(RMV(J+1)+RMV(J))*YSV(J)                               COMMENT   128
C-----Z-GRID.                                                           ST        74
      DO 103 K=2,NP1                                                    ST        75
103   ZDIF(K)=Z(K)-Z(K-1)                                               ST        76
      DO 113 K=2,N                                                      ST        77
113   ZS(K)=0.5*(Z(K+1)-Z(K-1))                                         ST        78
      ZS(2)=ZS(2)+0.5*ZDIF(2)                                           ST        79
      ZS(N) = ZS(N)+0.5*ZDIF(NP1)                                       ST        80
      ZS(NP1)=ZS(2)                                                     ST        81
      DO 123 K=3,N                                                      ST        82
      ZSW(K)=ZDIF(K)                                                    ST        83
      FZP(K)=ZDIF(K)/(2.*ZS(K))                                         ST        84
123   FZM(K)=1.-FZP(K)
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      ZSW(NP1)=ZDIF(2)+ZDIF(NP1)                                        ST        85
      FZP(NP1)=ZDIF(2)/ZS(NP1)                                          ST        86
      FZM(NP1)=1.-FZP(NP1)                                              ST        87
      FZP(2)=ZDIF(2)/ZS(2)                                              ST        88
      FZM(2)=1.-FZP(2)                                                  ST        89
C-----BOUNDARY CONDITION INDICES.                                       COMMENT   129
      DO 290 I=1,LP1                                                    ST        90
      IP=MIND(I+1,LP1)                                                  ST        91
      IL=MAXO(I-1,1)                                                    ST        92
      JWLI(I,1)=MAXO(JWLI(I,4),JWLI(IL,4))                             ST        93
      JWLI(I,2)=JWLI(I,4)+1                                             ST        94
      JWLI(I,3)=JWLI(I,4)                                               ST        95
      JWLI(I,5)=MIND(JWLI(IP,4),JWLI(I,4),JWLI(IL,4))                  ST        96
      JWLO(I,1)=MIND(JWLO(I,4),JWLO(IL,4))                             ST        97
      JWLO(I,2)=JWLO(I,4)                                               ST        98
      JWLO(I,3)=JWLO(I,4)                                               ST        99
      JWLO(I,5)=MAXO(JWLO(IP,4),JWLO(I,4),JWLO(IL,4))                  ST       100
  290 CONTINUE                                                          ST       101
      DO 292 J=1,NP1                                                    ST       102
      JP=MIND(J+1,NP1)                                                  ST       103
      JL=MAXO(J-1,1)                                                    ST       104
      IWLI(J,1)=IWLI(J,4)+1                                             ST       105
      IWLI(J,2)=MAXO(IWLI(J,4),IWLI(JL,4))                             ST       106
      IWLI(J,3)=IWLI(J,4)                                               ST       107
      IWLI(J,5)=MIND(IWLI(JP,4),IWLI(J,4),IWLI(JL,4))-1                ST       108
      IWLO(J,1)=IWLO(J,4)                                               ST       109
      IWLO(J,2)=MIND(IWLO(J,4),IWLO(JL,4))                             ST       110
      IWLO(J,3)=IWLO(J,4)                                               ST       111
      IWLO(J,5)=MAXO(IWLO(JP,4),IWLO(J,4),IWLO(JL,4))+1                ST       112
  292 CONTINUE                                                          ST       113
      RETURN                                                            ST       114
C  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  * ST       115
      ENTRY STRID2                                                      ST       116
C-----ENTRY STRID2 IS USED TO CALCULATE THE FINITE-DIFFERENCE           COMMENT   130
C     COEFFICIENTS AXP, AXM, AYP, AYM, AZP, AND AZM.                    COMMENT   131
C                                                                       COMMENT   132
C +-+-+-+-+-+-+-+-+-+-+-+-+-+-   U-VELOCITY   +-+-+-+-+-+-+-+-+-+-+-+-+-+- ST       117
      DO 360 LP=1,NINJNK                                                ST       118
  360 DU(LP)=0.0                                                        ST       119
      IF(ISOLVE(1)) 303,302,303                                         ST       120
303   IF(MOD(ISTEP,ISOLVE(1))) 302,304,302                              ST       121
304   CONTINUE                                                          ST       122
      ISTR=3                                                            ST       123
      JSTR=2                                                            ST       124
      KSTR=2                                                            ST       125
      NV=1                                                              ST       126
      NGOTO=1                                                           ST       127
C-----OBTAIN DIFFUSION COEFFICIENTS.                                    COMMENT   133
      CALL GAMMA                                                        ST       128
      DO 30 J=2,N                                                       ST       129
      IS=IWLI(J,NGOTO)                                                  ST       130
      IE=IWLO(J,NGOTO)                                                  ST       131
      TZFAC=R(J)/(R(N)+DFAC*(R(J)-R(N)))                                ST       132
      DO 30 I=IS,IE                                                     ST       133
      LP=JN(J)+I                                                        ST       134
      LZP=LP+NINJ                                                       ST       135
      LP11=LP-1                                                         ST       136
      LZP1=LZP-1                                                        ST       137
      AREA=RSU(I)*YS(J)                                                 ST       138
      AL7=RHO(LP)*W(LZP)*AREA                                           ST       139
      AL71=RHO(LP11)*W(LZP1)*AREA                                       ST       140
      AL7=.5*(AL7+AL71)                                                 ST       141
      AL7=AL7/2.                                                        ST       142
      T7=.5*(GAM(LP)+GAM(LP11))*AREA*TZFAC/(ZSW(NP1)*R(J))              ST       143
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      T7=AMAX1(T7,ABS(ALZ))                                              ST        144
      CZU(LP)=2.*ALZ                                                     ST        145
   30 CZ(LP)=T7+ALZ                                                      ST        146
      DO 301 K=2,M                                                       ST        147
C-----OBTAIN SOURCE TERMS AND EVAPORATION RATES.                         COMMENT   134
      CALL SOURCE                                                        ST        148
      CALL SOMAS                                                         ST        149
      DO 31 I=3,L                                                        ST        150
      JS=JWLI(I,NGOTO)+1                                                 ST        151
      AREA=XSU(I)*ZS(K)*RM(JS)                                           ST        152
      LP=KM(K)+JM(JS)+I                                                  ST        153
      LYM=LP-NI                                                          ST        154
      LXM1=LYM-1                                                         ST        155
      LXM=LP-1                                                           ST        156
      IF (JWLI(I,4).EQ.JS-1) GO TO 150                                   ST        157
      ALY=.5*(RHO(LP)+RHO(LYM))*V(LP)*AREA                               ST        158
      TY=.5*(GAM(LP)+GAM(LYM))*AREA/YDIF(JS)                             ST        159
      GO TO 152                                                          ST        160
  150 ALY=RHO(LYM)*V(LP)*AREA                                            ST        161
      DIST=.5*YDIF(JS)                                                   ST        162
      IF (JS.EQ.2) DIST=YDIF(2)                                          ST        163
      TY=GAM(LYM)*AREA/DIST                                              ST        164
  152 IF (JWLI(I-1,4).EQ.JS-1) GO TO 154                                 ST        165
      ALY1=.5*(RHO(LXM)+RHO(LXM1))*V(LXM)*AREA                           ST        166
      TY1=.5*(GAM(LXM)+GAM(LXM1))*AREA/YDIF(JS)                          ST        167
      GO TO 156                                                          ST        168
  154 ALY1=RHO(LXM1)*V(LXM)*AREA                                         ST        169
      DIST=.5*YDIF(JS)                                                   ST        170
      IF (JS.EQ.2) DIST=YDIF(JS)                                         ST        171
      TY1=GAM(LXM1)*AREA/DIST                                            ST        172
  156 ALY=.5*(ALY+ALY1)                                                  ST        173
      TY=.5*(TY+TY1)                                                     ST        174
      TY=AMAX1(TY,-ALY)                                                  ST        175
      CYU(I)=ALY                                                         ST        176
   31 CY(I)=TY+ALY                                                       ST        177
      DO 32 J=2,M                                                        ST        178
      KJM=KM(K)+JM(J)                                                    ST        179
      AREA=YSP(J)*ZS(K)                                                  ST        180
      IS=IWLI(J,NGOTO)                                                   ST        181
      IE=IWLO(J,NGOTO)                                                   ST        182
      I=IS-1                                                             ST        183
      LXP=KJM+IS                                                         ST        184
      LP=LXP-1                                                           ST        185
      LXM=LP-1                                                           ST        186
  200 ALXM=RHO(LXM)*U(LP)*AREA                                           ST        187
      ALXP=0.                                                            ST        188
      TX=GAM(LXM)*AREA/XS(I)                                             ST        189
      CXU=ALXM                                                           ST        190
  202 TX=AMAX1(TX,ALXP)                                                  ST        191
      TX=AMAX1(TX,-ALXM)                                                 ST        192
      CX=TX+ALXM                                                         ST        193
      TZFAC=R(J)/(R(M)+DFAC*(R(J)-R(M)))                                 ST        194
      DO 32 I=IS,IE                                                      ST        195
      MAX=JWLO(I,NGOTO)-1                                                ST        196
      LIJ=JM(J)+I                                                        ST        197
      LP=KJM+I                                                           ST        198
      LXP=LP+1                                                           ST        199
      LYP=LP+NI                                                          ST        200
      LZP=LP+NINJ                                                        ST        201
      LP11=LP-1                                                          ST        202
      LYP1=LYP-1                                                         ST        203
      LZP1=LZP-1                                                         ST        204
      AXM(LIJ)=CX                                                        ST        205
      AYM(LIJ)=CY(I)                                                     ST        206
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      AZM(LIJ)=CZ(LIJ)                                                  ST      207
      AREA=YSR(J)*ZS(K)                                                 ST      208
      IF (I.EQ.IF) GO TO 33                                             ST      209
      ALX=RHO(LP)*AREA*(FXP(I)*U(LXP)+FXM(I)*U(LP))                     ST      210
      ALXP=FXP(I)*ALX                                                   ST      211
      ALXM=FXM(I)*ALX                                                   ST      212
      TX=GAM(LP)*AREA/XS(I)                                             ST      213
      CXUP=ALX                                                          ST      214
      GO TO 34                                                          ST      215
   33 ALXP=RHO(LXP)*U(LXP)*AREA                                         ST      216
      ALXM=0.                                                           ST      217
      TX=GAM(LXP)*AREA/XS(L)                                            ST      218
      CXUP=ALXP                                                         ST      219
   34 TX=AMAX1(TX,ALXP)                                                 ST      220
      TX=AMAX1(TX,-ALXM)                                                ST      221
      AXP(LIJ)=TX-ALXP                                                  ST      222
      CX=TX+ALXM                                                        ST      223
      DIVG(LIJ)=DIVG(LIJ)+CXUP-CXU                                      ST      224
      CXU=CXUP                                                          ST      225
      AREA=ZS(K)*XSU(I)*RM(J+1)                                         ST      226
      IF (J.EQ.MAX) GO TO 35                                            ST      227
      ALY=.25*(RHO(LP)+RHO(LYP))*V(LYP)*AREA                            ST      228
      ALY1=.25*(RHO(LP11)+RHO(LYP11))*V(LYP1)*AREA                      ST      229
      ALY=.5*(ALY+ALY1)                                                 ST      230
      TY=.25*(GAM(LP)+GAM(LYP)+GAM(LP11)+GAM(LYP11))*AREA/YDIF(J+1)     ST      231
      TY=AMAX1(TY,ABS(ALY))                                             ST      232
      CYUP=2.*ALY                                                       ST      233
      GO TO 36                                                          ST      234
   35 IF (JWLO(I,4).EQ.MAX+1) GO TO 157                                 ST      235
      ALY=.5*(RHO(LP)+RHO(LYP))*V(LYP)*AREA                             ST      236
      TY=.5*(GAM(LP)+GAM(LYP))*AREA/YDIF(MAX+1)                         ST      237
      GO TO 158                                                         ST      238
  157 ALY=RHO(LYP)*V(LYP)*AREA                                          ST      239
      DIST=.5*YDIF(MAX+1)                                               ST      240
      IF (MAX.EQ.M) DIST=YDIF(MP1)                                      ST      241
      TY=GAM(LYP)*AREA/DIST                                             ST      242
  158 IF (JWLO(I-1,4).EQ.MAX+1) GO TO 159                               ST      243
      ALY1=.5*(RHO(LP11)+RHO(LYP1))*V(LYP1)*AREA                        ST      244
      TY=.5*(GAM(LP11)+GAM(LYP1))*AREA/YDIF(MAX+1)                      ST      245
      GO TO 160                                                         ST      246
  159 ALY1=RHO(LYP1)*V(LYP1)*AREA                                       ST      247
      DIST=.5*YDIF(MAX+1)                                               ST      248
      IF (MAX.EQ.M) DIST=YDIF(MP1)                                      ST      249
      TY1=GAM(LYP1)*AREA/DIST                                           ST      250
  160 ALY=.5*(ALY+ALY1)                                                 ST      251
      TY=.5*(TY+TY1)                                                    ST      252
      TY=AMAX1(TY,ALY)                                                  ST      253
      CYUP=ALY                                                          ST      254
   36 AYP(LIJ)=TY-ALY                                                   ST      255
      CY(I)=TY+ALY                                                      ST      256
      DIVG(LIJ)=DIVG(LIJ)+CYUP-CYU(I)                                   ST      257
      CYU(I)=CYUP                                                       ST      258
      AREA=XSU(I)*YS(J)                                                 ST      259
      IF(K.EQ.N) GO TO 37                                               ST      260
      ALZ=.25*(RHO(LP)+RHO(LZP))*W(LZP)*AREA                            ST      261
      ALZ1=.25*(RHO(LP11)+RHO(LZP1))*W(LZP1)*AREA                       ST      262
      ALZ=.5*(ALZ+ALZ1)                                                 ST      263
      GAMLP=.25*(GAM(LP)+GAM(LZP)+GAM(LP11)+GAM(LZP1))                  ST      264
      TZ=GAMLP*AREA*IZFAC/(ZDIF(K+1)*R(J))                              ST      265
      TZ=AMAX1(TZ,ABS(ALZ))                                             ST      266
      CZUP=2.*ALZ                                                       ST      267
      GO TO 38                                                          ST      268
   37 ALZ=RHO(LZP)*W(LZP)*AREA                                          ST      269
      ALZ1=RHO(LZP1)*W(LZP1)*AREA                                       ST      270
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      ALZ=.5*(ALZ+ALZ1)                                                  ST        271
      ALZ=ALZ/2.                                                         ST        272
      TZ=.5*(GAM(LZP)+GAM(LZP1))*AREA*TZFAC/(ZSW(NP1)*R(J))              ST        273
      TZ=AMAX1(TZ,ABS(ALZ))                                              ST        274
      CZUP=2.*ALZ                                                        ST        275
   38 AZP(LIJ)=TZ-ALZ                                                    ST        276
      CZ(LIJ)=TZ+ALZ                                                     ST        277
      DIVG(LIJ)=DIVG(LIJ)+CZUP-CZU(LIJ)                                  ST        278
      CZU(LIJ)=CZUP                                                      ST        279
      VOL=XSU(I)*YSR(J)*ZS(K)                                            ST        280
      IF (I.EQ.IWLI(J,NGOTO).AND.I.GT.3) VOL=VOL*(1.+.5*XSU(I-1)/XSU(I)) ST        281
      IF (I.EQ.IWLO(J,NGOTO).AND.I.LT.L) VOL=VOL*(1.+.5*XSU(I+1)/XSU(I)) ST        282
      LXM=LP-1                                                           ST        283
39    RDT=0.                                                             ST        284
392   DIVG(LIJ)=AMAX1(RDT,DIVG(LIJ))                                     ST        285
      DU(LP)=VOL/YDIF(I)                                                 ST        286
      SU(LIJ)=SU(LIJ)*VOL+DU(LP)*(P(LXM)-P(LP))+DIVG(LIJ)*U(LP)          ST        287
      SP(LIJ)=SP(LIJ)*VOL-DIVG(LIJ)                                      ST        288
   32 CONTINUE                                                           ST        289
C-----SOURCE TERM MODIFICATIONS - BOUNDARY CONDITIONS.                   COMMENT   135
      CALL SOMOD                                                         ST        290
C-----SOLVE FINITE-DIFFERENCE EQUATIONS IN SOLVE1 AND SOLVE2.            COMMENT   136
      CALL SOLVE1                                                        ST        291
  301 CONTINUE                                                           ST        292
      CALL SOLVE2                                                        ST        293
      CALL FMOD                                                          ST        294
  302 CONTINUE                                                           ST        295
C +-+-+-+-+-+-+-+-+-+-+-+-+-+-   V-VELOCITY   +-+-+-+-+-+-+-+-+-+-+-+-+- ST        296
      DO 460 LP=1,NINJNK                                                 ST        297
  460 DV(LP)=0.0                                                         ST        298
      IF(ISOLVE(2)) 403,402,403                                          ST        299
403   IF(MOD(ISTEP,ISOLVE(2))) 402,404,402                               ST        300
404   CONTINUE                                                           ST        301
      ISTR=2                                                             ST        302
      JSTR=3                                                             ST        303
      KSTR=2                                                             ST        304
      NV=2                                                               ST        305
      NGOTO=2                                                            ST        306
C-----OBTAIN DIFFUSION COEFFICIENTS.                                     COMMENT   137
      CALL GAMMA                                                         ST        307
      DO 40 J=3,M                                                        ST        308
      IS=IWLI(J,NGOTO)                                                   ST        309
      IF=IWLO(J,NGOTO)                                                   ST        310
      TZFAC=PR(J)/(PR(M)*DFAC*(RM(J)-RM(M)))                             ST        311
      DO 40 I=IS,IF                                                      ST        312
      LP=JM(J)+I                                                         ST        313
      LZP=LP+NINJ                                                        ST        314
      LP11=LP-NI                                                         ST        315
      LZP1=LZP-NI                                                        ST        316
      AREA=XS(I)*YSV(J)                                                  ST        317
      ALZ=RHO(LP)*W(LZP)*AREA                                            ST        318
      ALZ1=RHO(LP11)*W(LZP1)*AREA                                        ST        319
      ALZ=.5*(ALZ+ALZ1)                                                  ST        320
      ALZ=ALZ/2.                                                         ST        321
      TZ=.5*(GAM(LP)+GAM(LP11))*AREA*TZFAC/(ZSW(NP1)*RM(J))              ST        322
      TZ=AMAX1(TZ,ABS(ALZ))                                              ST        323
      CZU(LP)=2.*ALZ                                                     ST        324
   40 CZ(LP)=TZ+ALZ                                                      ST        325
      DO 401 K=2,M                                                       ST        326
C-----OBTAIN SOURCE TERMS AND EVAPORATION RATES.                         COMMENT   138
      CALL SOURCE                                                        ST        327
      CALL SOMAS                                                         ST        328
      DO 41 I=2,L                                                        ST        329
      J=JWLI(I,NGOTO)                                                    ST        330
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      AREA=ZS(K)*XS(I)*RMV(J+1)                                          ST      331
      LP=KM(K)+JM(J)+I                                                   ST      332
      LYP=LP+NI                                                          ST      333
      LYM=LP-NI                                                          ST      334
  206 ALYM=RHO(LYM)*V(LP)*AREA                                           ST      335
      ALYP=0.                                                            ST      336
      TY=GAM(LYM)*AREA/YS(J)                                             ST      337
      CYU(I)=ALYM                                                        ST      338
  208 TY=AMAX1(TY,ALYP)                                                  ST      339
      TY=AMAX1(TY,-ALYM)                                                 ST      340
   41 CY(I)=TY+ALYM                                                      ST      341
      DO 42 J=2,M                                                        ST      342
      KJM=KM(K)+JM(J)                                                    ST      343
      IS=IWLI(J,NGOTO)                                                   ST      344
        IE=IWLO(J,NGOTO)                                                 ST      345
      LXP=KJM+IS                                                         ST      346
      LP=LXP-1                                                           ST      347
      LP11=LP-NI                                                         ST      348
      LXP1=LXP-NI                                                        ST      349
      AREA=YSVR(J)*ZS(K)                                                 ST      350
      IF (IWLI(J,4).EQ.IS) GO TO 162                                     ST      351
      ALX=.5*(RHO(LP)+RHO(LXP))*U(LXP)*AREA                              ST      352
      TX=.5*(GAM(LP)+GAM(LXP))*AREA/XDIF(IS)                             ST      353
      GO TO 163                                                          ST      354
  162 ALX=RHO(LP)*U(LXP)*AREA                                            ST      355
      DIST=.5*XDIF(IS)                                                   ST      356
      IF (IS.EQ.2) DIST=XDIF(2)                                          ST      357
      TX=GAM(LP)*AREA/DIST                                               ST      358
  163 IF (IWLI(J-1,4).EQ.IS) GO TO 164                                   ST      359
      ALX1=.5*(RHO(LP11)+RHO(LXP1))*U(LXP1)*AREA                         ST      360
      TX1=.5*(GAM(LP11)+GAM(LXP1))*AREA/XDIF(IS)                         ST      361
      GO TO 165                                                          ST      362
  164 ALX1=RHO(LP11)*U(LXP1)*AREA                                        ST      363
      DIST=.5*XDIF(IS)                                                   ST      364
      IF (IS.EQ.2) DIST=XDIF(2)                                          ST      365
      TX1=GAM(LP11)*AREA/DIST                                            ST      366
  165 ALX=.5*(ALX+ALX1)                                                  ST      367
      TX=.5*(TX+TX1)                                                     ST      368
      TX=AMAX1(TX,-ALX)                                                  ST      369
      CYU=ALX                                                            ST      370
      CX=TX+ALX                                                          ST      371
      TZFAC=RM(J)/(RM(M)+DFAC*(RM(J)-RM(M)))                             ST      372
      DO 42 I=IS,IE                                                      ST      373
      MAX=JWLO(I,NGOTO)-1                                                ST      374
      LIJ=JM(J)+I                                                        ST      375
      LP=KJM+I                                                           ST      376
      LXP=LP+1                                                           ST      377
      LYP=LP+NI                                                          ST      378
      LZP=LP+NINJ                                                        ST      379
      LP11=LP-NI                                                         ST      380
      LXP1=LXP-NI                                                        ST      381
      LZP1=LZP-NI                                                        ST      382
      AXM(LIJ)=CX                                                        ST      383
      AYM(LIJ)=CY(I)                                                     ST      384
      AZM(LIJ)=CZ(LIJ)                                                   ST      385
      AREA=YSVR(J)*ZS(K)                                                 ST      386
      IF (I.EQ.IE) GO TO 43                                              ST      387
      ALX=.25*(RHO(LP)+RHO(LXP))*U(LXP)*AREA                             ST      388
      ALX1=.25*(RHO(LP11)+RHO(LXP1))*U(LXP1)*AREA                        ST      389
      ALX=.5*(ALX+ALX1)                                                  ST      390
      TX=.25*(GAM(LP)+GAM(LXP)+GAM(LP11)+GAM(LXP1))*AREA/XDIF(I+1)       ST      391
      TX=AMAX1(TX,ABS(ALX))                                              ST      392
      CYUP=2.*ALX                                                        ST      393
      GO TO 44                                                           ST      394
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   43 IF (IWLO(J,4).EQ.IE) GO TO 167                                    ST      395
      ALX=.5*(RHO(LP)+RHO(LXP))*U(LXP)*AREA                             ST      396
      TX=.5*(GAM(LP)+GAM(LXP))*AREA/XDIF(I+1)                           ST      397
      GO TO 168                                                         ST      398
  167 ALX=RHO(LXP)*U(LXP)*AREA                                          ST      399
      DIST=.5*XDIF(I+1)                                                 ST      400
      IF (I.EQ.L) DIST=XDIF(LP1)                                        ST      401
      TX=GAM(LXP)*AREA/DIST                                             ST      402
  168 IF (IWLO(J-1,4).EQ.IE) GO TO 169                                  ST      403
      ALX1=.5*(RHO(LP11)+RHO(LXP1))*U(LXP1)*AREA                        ST      404
      TX1=.5*(GAM(LP11)+GAM(LXP1))*AREA/XDIF(I+1)                       ST      405
      GO TO 170                                                         ST      406
  169 ALX1=RHO(LXP1)*U(LXP1)*AREA                                       ST      407
      DIST=.5*XDIF(I+1)                                                 ST      408
      IF (I.EQ.L) DIST=XDIF(LP1)                                        ST      409
      TX1=GAM(LXP1)*AREA/DIST                                           ST      410
  170 ALX=.5*(ALX+ALX1)                                                 ST      411
      TX=.5*(TX+TX1)                                                    ST      412
      TX=AMAX1(TX,ALX)                                                  ST      413
      CXUP=ALX                                                          ST      414
   44 AXP(LIJ)=TX-ALX                                                   ST      415
      CX=TX+ALX                                                         ST      416
      DIVG(LIJ)=DIVG(LIJ)+CXUP-CXU                                      ST      417
      CXU=CXUP                                                          ST      418
      AREA=ZS(K)*XS(I)*RMV(J+1)                                         ST      419
      IF (J.EQ.JWLO(I,NGOTO)-1) GO TO 45                                ST      420
      ALY=RHO(LP)*AREA*(FYP(J)*V(LYP)+FYM(J)*V(LP))                     ST      421
      ALYP=FYP(J)*ALY                                                   ST      422
      ALYM=FYM(J)*ALY                                                   ST      423
      TY=GAM(LP)*AREA/YS(J)                                             ST      424
      CYUP=ALY                                                          ST      425
      GO TO 46                                                          ST      426
   45 ALYP=RHO(LYP)*V(LYP)*AREA                                         ST      427
      ALYM=0.                                                           ST      428
      TY=GAM(LYP)*AREA/YS(J)                                            ST      429
      CYUP=ALYP                                                         ST      430
   46 TY=AMAX1(TY,ALYP)                                                 ST      431
      TY=AMAX1(TY,-ALYM)                                                ST      432
      AYP(LIJ)=TY-ALYP                                                  ST      433
      CY(I)=TY+ALYM                                                     ST      434
      DIVG(LIJ)=DIVG(LIJ)+CYUP-CYU(I)                                   ST      435
      CYU(I)=CYUP                                                       ST      436
      AREA=XS(I)*YSV(J)                                                 ST      437
      IF(K.EQ.N) GO TO 47                                               ST      438
      ALZ=.25*(RHO(LP)+RHO(LZP))*W(LZP)*AREA                            ST      439
      ALZ1=.25*(RHO(LP11)+RHO(LZP1))*W(LZP1)*AREA                       ST      440
      ALZ=.5*(ALZ+ALZ1)                                                 ST      441
      GAMLP=.25*(GAM(LP)+GAM(LZP)+GAM(LP11)+GAM(LZP1))                  ST      442
      TZ=GAMLP*AREA*TZFAC/(ZDIF(K+1)*RM(J))                             ST      443
      TZ=AMAX1(TZ,ABS(ALZ))                                             ST      444
      CZUP=2.*ALZ                                                       ST      445
      GO TO 48                                                          ST      446
   47 ALZ=RHO(LZP)*W(LZP)*AREA                                          ST      447
      ALZ1=RHO(LZP1)*W(LZP1)*AREA                                       ST      448
      ALZ=.5*(ALZ+ALZ1)                                                 ST      449
      ALZ=ALZ/2.                                                        ST      450
      TZ=GAM(LZP)*AREA*TZFAC/(ZSW(NP1)*RM(J))                           ST      451
      TZ=AMAX1(TZ,ABS(ALZ))                                             ST      452
      CZUP=2.*ALZ                                                       ST      453
   48 AZP(LIJ)=TZ-ALZ                                                   ST      454
      CZ(LIJ)=TZ+ALZ                                                    ST      455
      DIVG(LIJ)=DIVG(LIJ)+CZUP-CZU(LIJ)                                 ST      456
      CZU(LIJ)=CZUP                                                     ST      457
      VOL=XS(I)*YSVR(J)*ZS(K)                                           ST      458
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      IF (J.EQ.JWLI(I,NGOTO).AND.J.GT.3) VOL=VOL*(1.+.5*YSVR(J-1)/      ST        459
     1  YSVR(J))                                                        ST        460
      IF (J.EQ.JWLO(I,NGOTO).AND.J.LT.M) VOL=VOL*(1.+.5*YSVR(J+1)/      ST        461
     1  YSVR(J))                                                        ST        462
      LYM=LP-NI                                                        ST        463
49    ROT=0.                                                           ST        464
492   DIVG(LIJ)=AMAX1(ROT,DIVG(LIJ))                                   ST        465
      DV(LP)=VOL/YDIF(J)                                               ST        466
      SU(LIJ)=SU(LIJ)*VOL+DV(LP)*(P(LYM)-P(LP))+DIVG(LIJ)*V(LP)        ST        467
      SP(LIJ)=SP(LIJ)*VOL-DIVG(LIJ)                                    ST        468
      SU(LIJ)=SU(LIJ)+PLAXM1*0.5*(RHO(LP)+RHO(LP-NI))*(0.25*(W(LP)+W(LP+ ST        469
     1NINJ)+W(LP+NINJ-NI)+W(LP-NI)))**2*VOL/RM(J)                      ST        470
   42 CONTINUE                                                         ST        471
C-----SOURCE TERM MODIFICATIONS - BOUNDARY CONDITIONS.                 COMMENT   139
      CALL SOMOD                                                       ST        472
C-----SOLVE FINITE-DIFFERENCE EQUATIONS IN SOLVE1 AND SOLVE2.          COMMENT   140
      CALL SOLVE1                                                      ST        473
  401 CONTINUE                                                         ST        474
      CALL SOLVE2                                                      ST        475
      CALL FMOD                                                        ST        476
  402 CONTINUE                                                         ST        477
C +-+-+-+-+-+-+-+-+-+-+-+-+-+-+    W-VELOCITY    +-+-+-+-+-+-+-+-+-+-+-+-+-+- ST        478
      DO 505 LP=1,NINJNK                                               ST        479
  505 DW(LP)=0.0                                                       ST        480
      IF(ISOLVE(3)) 503,502,503                                        ST        481
503   IF(MOD(ISTEP,ISOLVE(3))) 502,504,502                             ST        482
504   CONTINUE                                                         ST        483
      ISTR=2                                                           ST        484
      JSTR=2                                                           ST        485
      KSTR=3                                                           ST        486
      NV=3                                                             ST        487
      NGOTO=3                                                          ST        488
C-----OBTAIN DIFFUSION COEFFICIENTS.                                   COMMENT   141
      CALL GAMMA                                                       ST        489
      DO 50 J=2,M                                                      ST        490
      IS=IWLI(J,NGOTO)                                                 ST        491
      IE=IWLO(J,NGOTO)                                                 ST        492
      TZFAC=1.0                                                        ST        493
      DO 50 I=IS,IE                                                    ST        494
      LIJ=JM(J)+I                                                      ST        495
      LP=KM(2)+LIJ                                                     ST        496
      LZP=LP+NINJ                                                      ST        497
      AREA=XS(I)*YS(J)                                                 ST        498
      ALZ=RHO(LP)*AREA*(FZP(2)*W(LZP)+FZM(2)*W(LP))                    ST        499
      ALZP=FZP(2)*ALZ                                                  ST        500
      ALZM=FZM(2)*ALZ                                                  ST        501
      TZ=GAM(LP)*AREA*TZFAC/(ZS(2)*R(J))                               ST        502
      CZU(LIJ)=ALZ                                                     ST        503
      TZ=AMAX1(TZ,ALZP)                                                ST        504
      TZ=AMAX1(TZ,-ALZM)                                               ST        505
   50 CZ(LIJ)=TZ+ALZM                                                  ST        506
      DO 901 K=3,NP1                                                   ST        507
C-----OBTAIN SOURCE TERMS AND EVAPORATION RATES.                       COMMENT   142
      CALL SOURCE                                                      ST        508
      CALL SOMAS                                                       ST        509
      DO 51 I=2,L                                                      ST        510
      J=JWLI(I,NGOTO)+1                                                ST        511
      LP=KM(K)+JM(J-1)+I                                               ST        512
      LYP=LP+NI                                                        ST        513
      LP11=LP-NINJ                                                     ST        514
      LYP1=LYP-NINJ                                                    ST        515
      APEA=ZSW(K)*XS(I)*RM(J)                                          ST        516
      ALY=RHO(LP)*V(LYP)*AREA                                          ST        517
      ALY1=RHO(LP11)*V(LYP1)*AREA                                      ST        518
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```
      ALY=.5*(ALY+ALY1)                                                  ST      519
      DIST=.5*YDIF(J)                                                    ST      520
      IF (J.EQ.2) DIST=YDIF(2)                                           ST      521
      TY=.5*(GAM(LP)+GAM(LP11))*AREA/DIST                                ST      522
      TY=AMAX1(TY,-ALY)                                                  ST      523
      CYU(I)=ALY                                                         ST      524
   91 CY(I)=TY+ALY                                                       ST      525
      DO 92 J=2,M                                                        ST      526
      KJM=KM(K)+JM(J)                                                    ST      527
      IS=IWL(I,NGOTO)                                                    ST      528
      IF=IWL(I,NGOTO)                                                    ST      529
      LXP=KJM+IS                                                         ST      530
      LP=LXP-1                                                           ST      531
      LP11=LP-NINJ                                                       ST      532
      LXP1=LXP-NINJ                                                      ST      533
      AREA=YSR(J)*ZSW(K)                                                 ST      534
      ALX=RHO(LP)*U(LXP)*AREA                                            ST      535
      ALX1=RHO(LP11)*U(LXP1)*AREA                                        ST      536
      ALX=.5*(ALX+ALX1)                                                  ST      537
      DIST=.5*XDIF(IS)                                                   ST      538
      IF (IS.EQ.2) DIST=XDIF(2)                                          ST      539
      TX=.5*(GAM(LP)+GAM(LP11))*AREA/DIST                                ST      540
      TX=AMAX1(TX,-ALX)                                                  ST      541
      CXU=ALX                                                            ST      542
      CX=TX+ALX                                                          ST      543
      TZFAC=1.0                                                          ST      544
      DO 52 I=IS,IF                                                      ST      545
      MAX=JWL(I,NGOTO)-1                                                 ST      546
      LIJ=JM(J)+I                                                        ST      547
      LP=KJM+I                                                           ST      548
      LXP=LP+1                                                           ST      549
      LYP=LP+NI                                                          ST      550
      LZP=LP+NINJ                                                        ST      551
      LP11=LP-NINJ                                                       ST      552
      LXP1=LXP-NINJ                                                      ST      553
      LYP1=LYP-NINJ                                                      ST      554
      AXM(LIJ)=CX                                                        ST      555
      AYM(LIJ)=CY(I)                                                     ST      556
      AZM(LIJ)=CZ(LIJ)                                                   ST      557
      AREA=YSR(J)*ZSW(K)                                                 ST      558
      IF (I.EQ.IF) GO TO 53                                              ST      559
      ALX=.25*(RHO(LP)+RHO(LXP))*U(LXP)*AREA                             ST      560
      ALX1=.25*(RHO(LP11)+RHO(LXP1))*U(LXP1)*AREA                        ST      561
      ALX=.5*(ALX+ALX1)                                                  ST      562
      TX=.25*(GAM(LP)+GAM(LXP)+GAM(LP11)+GAM(LXP1))*AREA/XDIF(I+1)       ST      563
      TX=AMAX1(TX,ABS(ALX))                                              ST      564
      CXUP=2.*ALX                                                        ST      565
      GO TO 54                                                           ST      566
   53 ALX=RHO(LXP)*U(LXP)*AREA                                           ST      567
      ALX1=RHO(LXP1)*U(LXP1)*AREA                                        ST      568
      ALX=.5*(ALX+ALX1)                                                  ST      569
      DIST=.5*XDIF(I+1)                                                  ST      570
      IF (I.EQ.1) DIST=XDIF(LP1)                                         ST      571
      TX=.5*(GAM(LXP)+GAM(LXP1))*AREA/DIST                               ST      572
      TX=AMAX1(TX,ALX)                                                   ST      573
      CXUP=ALX                                                           ST      574
   54 AXP(LIJ)=TX-ALX                                                    ST      575
      CX=TX+ALX                                                          ST      576
      DIVG(LIJ)=DIVG(LIJ)+CXUP-CXU                                       ST      577
      CXU=CXUP                                                           ST      578
      AREA=ZSW(K)*RS(I)*RM(J+1)                                          ST      579
      IF (J.EQ.MAX) GO TO 55                                             ST      580
      ALY=.25*(RHO(LP)+RHO(LYP))*V(LYP)*AREA                             ST      581
      ALY1=.25*(RHO(LP11)+RHO(LYP1))*V(LYP1)*AREA                        ST      582
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      ALY=.5*(ALY+ALY1)                                                  ST      583
      TY=.25*(GAM(LP)+GAM(LYP)+GAM(LP11)+GAM(LYP1))*AREA/YDIF(J+1)       ST      584
      TY=AMAX1(TY,ABS(ALY))                                              ST      585
      CYUP=2.*ALY                                                        ST      586
      GO TO 56                                                           ST      587
   55 ALY=RHO(LYP)*V(LYP)*AREA                                           ST      588
      ALY1=RHO(LYP1)*V(LYP1)*AREA                                        ST      589
      ALY=.5*(ALY+ALY1)                                                  ST      590
      DIST=.5*YDIF(J+1)                                                  ST      591
      IF (J.EQ.M) DIST=YDIF(MP1)                                         ST      592
      TY=.5*(GAM(LYP)+GAM(LYP1))*AREA/DIST                               ST      593
      TY=AMAX1(TY,ALY)                                                   ST      594
      CYUP=ALY                                                           ST      595
   56 AYP(LIJ)=TY-ALY                                                    ST      596
      CY(I)=TY+ALY                                                       ST      597
      DIVG(LIJ)=DIVG(LIJ)+CYUP-CYU(I)                                    ST      598
      CYU(I)=CYUP                                                        ST      599
      AREA=XS(I)*YS(J)                                                   ST      600
      DENSTY=RHO(LP)                                                     ST      601
      IF(K.EQ.NP1) DENSTY=RHO(LIJ+NINJ)                                  ST      602
      IF (K.EQ.NP1) WLZP=W(LIJ+2*NINJ)                                   ST      603
      IF(K.LT.NP1) WLZP=W(LZP)                                           ST      604
      ALZ=DENSTY*AREA*(FZP(K)*WLZP+FZM(K)*W(LP))                         ST      605
      ALZP=FZP(K)*ALZ                                                    ST      606
      ALZM=FZM(K)*ALZ                                                    ST      607
      TZ=GAM(LP)*AREA*TZFAC/(ZS(K)*R(J))                                 ST      608
      CZUP=ALZ                                                           ST      609
      TZ=AMAX1(TZ,ALZP)                                                  ST      610
      TZ=AMAX1(TZ,-ALZM)                                                 ST      611
      AZP(LIJ)=TZ-ALZP                                                   ST      612
      CZ(LIJ)=TZ+ALZM                                                    ST      613
      DIVG(LIJ)=DIVG(LIJ)+CZUP-CZU(LIJ)                                  ST      614
      CZU(LIJ)=CZUP                                                      ST      615
      VOL=XS(I)*YSR(J)*ZSW(K)                                            ST      616
      L7M=LP-NINJ                                                        ST      617
   59 ROT=0.                                                             ST      618
  592 DIVG(LIJ)=AMAX1(ROT,DIVG(LIJ))                                     ST      619
      DW(LP)=VOL/ZDIF(K)/R(J)                                            ST      620
      IF (K.EQ.NP1) DW(LP)=DW(LP)*ZDIF(K)/ZSW(K)                         ST      621
      SU(LIJ)=SU(LIJ)+VOL*DW(LP)*(P(LZM)-P(LP))+DIVG(LIJ)*W(LP)          ST      622
      SP(LIJ)=SP(LIJ)+VOL-DIVG(LIJ)                                      ST      623
      IF(IPLAX.EQ.1)GO TO 52                                             NASAX    37
      RVAV=0.125*(RHO(LP)+RHO(LP-NINJ))*(V(LP)+V(LP-NINJ)+V(LP+NI)       NASAX    38
     1+V(LP-NINJ+NI))*VOL/R(J)                                           NASAX    39
      IF(RVAV.LT.0.0)GO TO 57                                            NASAX    40
      SP(LIJ)=SP(LIJ)-RVAV                                               NASAX    41
      GO TO 52                                                           NASAX    42
   57 SU(LIJ)=SU(LIJ)-RVAV*W(LP)                                         NASAX    43
   52 CONTINUE                                                           ST      626
C-----SOURCE TERM MODIFICATIONS - BOUNDARY CONDITIONS.                   COMMENT 143
      CALL SCMOD                                                         ST      627
C-----SOLVE FINITE-DIFFERENCE EQUATIONS IN SOLVE1 AND SOLVE2.            COMMENT 144
      CALL SOLVE1                                                        ST      628
  501 CONTINUE                                                           ST      629
      CALL SOLVE2                                                        ST      630
  502 CONTINUE                                                           ST      631
      CALL VELMOD                                                        ST      632
C +-+-+-+-+-+-+-+-+-+-+-+-+-   PRESSURE PERTABATION EQUATION  +-+-+-+-+-+-+-+-+-+ ST      633
      NGOTO=4                                                            ST      634
      IF(ISOLVE(4)) 603,602,603                                          ST      635
  603 IF(MOD(ISTEP,ISOLVE(4))) 602,604,602                               ST      636
  604 CONTINUE                                                           ST      637
      DO 605 LP=1,NINJMK                                                 ST      638
  605 PP(LP)=0.0                                                         ST      639
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      ISTR=2                                                            ST        640
      JSTR=2                                                            ST        641
      KSTR=2                                                            ST        642
      NV=4                                                              ST        643
 6000 CONTINUE                                                          ST        644
CALCULATE CONTINUITY ERRORS.                                            COMMENT   145
      DO 60 J=2,P                                                       ST        645
      IS=IWLI(J,NGOTO)                                                  ST        646
      IE=IWLF(J,NGOTO)                                                  ST        647
      DO 60 I=IS,IE                                                     ST        648
      LP=JP(J)+I                                                        ST        649
      LZP=LP+NINJ                                                       ST        650
      RHOA=RHO(LP)*XS(I)*YS(J)                                          ST        651
      CZU(LP)=RHOA*DW(LZP)                                              ST        652
   60 CZ(LP)=RHOA*DW(LZP)                                               ST        653
      DO 601 K=2,N                                                      ST        654
      DO 61 I=2,L                                                       ST        655
      J=JWLI(I,NGOTO)+1                                                 ST        656
      LP=KN(K)+JP(J-1)+I                                                ST        657
      LYP=LP+NI                                                         ST        658
      RHOA=RHO(LP)*ZS(K)*XS(I)*RM(J)                                    ST        659
      CYU(I)=RHOA*V(LYP)                                                ST        660
   61 CY(I)=RHOA*DV(LYP)                                                ST        661
      DO 62 J=2,M                                                       ST        662
      KJM=KM(K)+JP(J)                                                   ST        663
      IS=IWLI(J,NGOTO)                                                  ST        664
      IE=IWLO(J,NGOTO)                                                  ST        665
      LP=KJM+IS-1                                                       ST        666
      LXP=LP+1                                                          ST        667
      RHOA=RHO(LP)*YSR(J)*ZS(K)                                         ST        668
      CXU=RHOA*U(LXP)                                                   ST        669
      CX=RHOA*DU(LXP)                                                   ST        670
      DO 62 I=IS,IE                                                     ST        671
      MAX=JWLO(I,NGOTO)-1                                               ST        672
      LIJ=JP(J)+I                                                       ST        673
      LP=KJM+I                                                          ST        674
      LXP=LP+1                                                          ST        675
      LYP=LP+NI                                                         ST        676
      LZP=LP+NINJ                                                       ST        677
      AXM(LIJ)=CX                                                       ST        678
      AYM(LIJ)=CY(I)                                                    ST        679
      AZM(LIJ)=CZ(LIJ)                                                  ST        680
      IF (I.EQ.IE) GO TO 63                                             ST        681
      RHOA=0.5*(RHO(LP)+RHO(LXP))*YSR(J)*ZS(K)                          ST        682
      GO TO 64                                                          ST        683
63    RHOA=RHO(LXP)*YSR(J)*ZS(K)                                        ST        684
   64 CX=RHOA*DU(LXP)                                                   ST        685
      CXUP=RHOA*U(LXP)                                                  ST        686
      SU(LIJ)=CXU-CXUP                                                  ST        687
      CXU=CXUP                                                          ST        688
      AXP(LIJ)=CX                                                       ST        689
      IF (J.EQ.MAX) GO TO 65                                            ST        690
      RHOA=0.5*(RHO(LP)+RHO(LYP))*ZS(K)*XS(I)*RM(J+1)                   ST        691
      GO TO 66                                                          ST        692
   65 RHOA=RHO(LYP)*ZS(K)*XS(I)*RM(J+1)                                 ST        693
   66 CY(I)=RHOA*DV(LYP)                                                ST        694
      CYUP=RHOA*V(LYP)                                                  ST        695
      SU(LIJ)=SU(LIJ)+CYU(I)-CYUP                                       ST        696
      CYU(I)=CYUP                                                       ST        697
      AYP(LIJ)=CY(I)                                                    ST        698
      IF(K.EQ.N) GO TO 67                                               ST        699
      RHOA=0.5*(RHO(LP)+RHO(LZP))*XS(I)*YS(J)                           ST        700
      GO TO 68                                                          ST        701
67    RHOA=RHO(LZP)*XS(I)*YS(J)                                         ST        702
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   68 CZ(LIJ)=RHOA*DW(LZP)
      CZUP=RHOA*W(LZP)                                                  ST        703
      SU(LIJ)=SU(LIJ)+CZU(LIJ)-CZUP                                     ST        704
      CZU(LIJ)=CZUP                                                     ST        705
      AZP(LIJ)=CZ(LIJ)                                                  ST        706
      SP(LIJ)=0.                                                        ST        707
   62 CONTINUE                                                          ST        708
C-----SOURCE TERM MODIFICATIONS - BOUNDARY CONDITIONS.                   ST        709
      CALL SOMOD                                                        COMMENT   146
C-----SOLVE FINITE-DIFFERENCE EQUATIONS IN SOLVE1 AND SOLVE2.            ST        710
      CALL SOLVE1                                                       COMMENT   147
  601  CONTINUE                                                         ST        711
      CALL SOLVE2                                                       ST        712
  602 CONTINUE                                                          ST        713
COME HERE TO CORRECT VELOCITIES AND PRESSURES                           ST        714
      CALL FPCO                                                         ST        715
      DO 620 K=2,NP1                                                    ST        716
      DO 620 J=2,MP1                                                    ST        717
      KJM=KM(K)+JM(J)                                                   ST        718
      IS=IWLI(J,NGOTO)                                                  ST        719
      IF=IWLO(J,NGOTO)+1                                                ST        720
      DO 620 I=IS,IF                                                    ST        721
      LP=KJM+I                                                          ST        722
      LXM=LP-1                                                          ST        723
      LYM=LP-NI                                                         ST        724
      LZM=LP-NINJ                                                       ST        725
      U(LP)=U(LP)+DU(LP)*(PP(LXM)-PP(LP))                               ST        726
      V(LP)=V(LP)+DV(LP)*(PP(LYM)-PP(LP))                               ST        727
      W(LP)=W(LP)+DW(LP)*(PP(LZM)-PP(LP))                               ST        728
  620 CONTINUE                                                          ST        729
      GO TO (621,622),IPAR                                              ST        730
  622 PLPREF=P(LPREF)+PP(LPREF)*RELAX(NP)                               ST        731
  621 CONTINUE                                                          ST        732
      DO 630 K=2,N                                                      ST        733
      DO 630 J=2,M                                                      ST        734
      KJM=KM(K)+JM(J)                                                   ST        735
      IS=IWLI(J,NGOTO)                                                  ST        736
      IF=IWLO(J,NGOTO)                                                  ST        737
      DO 630 I=IS,IF                                                    ST        738
      LP=KJM+I                                                          ST        739
      P(LP)=P(LP)+PP(LP)*RELAX(NP)                                      ST        740
      GO TO (631,632),IPAR                                              ST        741
  632 P(LP)=P(LP)-PLPREF                                                ST        742
  631 CONTINUE                                                          ST        743
  630 PP(LP)=0.                                                         ST        744
C-----CYCLIC BOUNDARY CONDITIONS.                                        ST        745
      DO 641 J=1,MP1                                                    COMMENT   148
      DO 641 I=1,LP1                                                    ST        746
      LPN=I+JM(J)+KM(NP1)                                               ST        747
      LP2=I+JM(J)+KM(2)                                                 ST        748
      P(LPN)=P(LP2)                                                     ST        749
  641 CONTINUE                                                          ST        750
      REWIND NTP2                                                       ST        751
      WRITE (NTP2) U,V,W,P                                              ST        752
C +-+-+-+-+-+-+-+-+-+-+-+-+-+-+-    F-VARIABLES    +-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+  ST  753
      DO 700 NV=5,NNV                                                   ST        754
      ICONVG=0                                                          ST        755
      NITER=ITNOX                                                       NOX       204
      IF(ISTEP+1.NE.LASTEP)NITER=1                                      NOX       205
      IF(NV.NE.LVH1)NITER=1                                             NOX       206
      DO 706 ITR=1,NITER                                                NOX       207
      IF (NV.NE.LVK) GO TO 710                                          NOX       208
      REWIND NTP1                                                       ST        756
      READ (NTP1)                                                       ST        757
                                                                        ST        758
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C  ----  HERE PP IS KE,  P IS DISSIPATION                    ST      759
      READ (NTP1) PP,P                                       ST      760
  710 IF (NV.NE.LVFUOK) GO TO 714                            ST      761
C -------- HERE PP IS KF, P IS DISS                          ST      762
      WRITE (NTP2) PP,P                                      ST      763
C -------- HERE PP IS PHI, P IS MFU, DU IS MCO               ST      764
      READ (NTP1) PP,P,DU                                    ST      765
  714 IF (NV.NE.LVH) GO Tu 720                               ST      766
C ------ HERE DV IS ENTHALPY, DW IS FAV                      ST      767
      READ (NTP1) DV,DW                                      ST      768
      ICPS=3                                                 NOX     209
      NS1=IDO2                                               NOX     210
      NS2=IDN2                                               NOX     211
      S2(IDO2)=RATIO2/SMW(IDO2)                              NOX     212
      S2(IDN2)=(1.0-RATIO2)/SMW(IDN2)                        NOX     213
C-----BOUNDARY VALUES OF ENTHALPY.                           COMMENT 149
      DO 716 K=1,NP1                                         ST      769
      DO 717 I=1,LP1                                         ST      770
      IF (IKIN(I,K).EQ.2.OR.IKIN(I,K).EQ.3) GO TO 712        ST      771
      LP=KM(K)+JM(JWLI(I,4))+I                               ST      772
      LPH=LP+NVM(NVH)                                        ST      773
      TK=TEMP(LP)                                            NOX     214
      TKINV=1.000/TK                                         NOX     215
      CALL HCPS                                              NOX     216
      F(LPH)=HSUM*UNICON*TK                                  NOX     217
  712 IF (IKIN(I,K).EQ.1.OR.IKIN(I,K).EQ.3) GO TO 717        ST      775
      LP=KM(K)+JM(JWLO(I,4))+I                               ST      776
      LPH=LP+NVM(NVH)                                        ST      777
      TK=TEMP(LP)                                            NOX     218
      TKINV=1.000/TK                                         NOX     219
      CALL HCPS                                              NOX     220
      F(LPH)=HSUM*UNICON*TK                                  NOX     221
  717 CONTINUE                                               ST      779
      DO 716 J=1,MP1                                         ST      780
      IF (JKIN(J,K).EQ.1) GO TO 760                          ST      781
      LP=KM(K)+JM(J)+IWLI(J,4)-1                             ST      782
      LPH=LP+NVM(NVH)                                        ST      783
      TK=TEMP(LP)                                            NOX     222
      TKINV=1.000/TK                                         NOX     223
      CALL HCPS                                              NOX     224
      F(LPH)=HSUM*UNICON*TK                                  NOX     225
  760 IF (J.GT.JWOI.AND.J.LT.JWOO) GO TO 716                 ST      785
      LP=KM(K)+JM(J)+IWLO(J,4)+1                             ST      786
      LPH=LP+NVM(NVH)                                        ST      787
      TK=TEMP(LP)                                            NOX     226
      TKINV=1.000/TK                                         NOX     227
      CALL HCPS                                              NOX     228
      F(LPH)=HSUM*UNICON*TK                                  NOX     229
  716 CONTINUE                                               ST      789
  720 IF (ISOLVE(NV)) 703,702,703                            ST      790
  703 IF (MOD(ISTEP,ISOLVE(NV))) 702,704,702                 ST      791
  704 CONTINUE                                               ST      792
      ISTR=2                                                 ST      793
      JSTR=2                                                 ST      794
      KSTR=2                                                 ST      795
C-----OBTAIN DIFFUSION COEFFICIENTS.                         COMMENT 150
      CALL GAMMA                                             ST      796
      DO 70 J=2,M                                            ST      797
      IS=IWLI(J,NGOTO)                                       ST      798
      IE=IWLO(J,NGOTO)                                       ST      799
      T2FAC=R(J)/(R(M)+DFAC*(R(J)-R(M)))                     ST      800
      DO 70 I=IS,IE                                          ST      801
      LP=JM(J)+I                                             ST      802
      L2P=LP+NINJ                                            ST      803
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      AREA=XS(I)*YS(J)                                                  ST        804
      ALZ=RHO(LP)*W(LZP)*AREA                                           ST        805
      ALZ=ALZ/2.                                                        ST        806
      TZ=GAM(LP)*AREA*TZFAC/(ZSW(NP1)*R(J))                             ST        807
      TZ=AMAX1(TZ,ABS(ALZ))                                             ST        808
      CZU(LP)=2.*ALZ                                                    ST        809
   70 CZ(LP)=TZ+ALZ                                                     ST        810
      DO 701 K=2,N                                                      ST        811
C-----OBTAIN SOURCE TERMS AND EVAPORATION RATES.                        COMMENT   151
      CALL SOURCE                                                       ST        812
      CALL SOMAS                                                        ST        813
      DO 71 I=2,L                                                       ST        814
      J=JWLI(I,NGOTO)+1                                                 ST        815
      LP=KR(K)+JM(J-1)+I                                                ST        816
      LYP=LP+NI                                                         ST        817
      AREA=ZS(K)*XS(I)*RM(J)                                            ST        818
      ALY=RHO(LP)*V(LYP)*AREA                                           ST        819
      DIST=.5*YDIF(J)                                                   ST        820
      IF (J.EQ.2) DIST=YDIF(2)                                          ST        821
      TY=GAM(LP)*AREA/DIST                                              ST        822
       TY=AMAX1(TY,-ALY)                                                ST        823
      CYU(I)=ALY                                                        ST        824
   71 CY(I)=TY+ALY                                                      ST        825
      DO 72 J=2,M                                                       ST        826
      KJM=KM(K)+JM(J)                                                   ST        827
      IS=IWLI(J,NGOTO)                                                  ST        828
      IE=IWLO(J,NGOTO)                                                  ST        829
      LXP=KJM+IS                                                        ST        830
      LP=LXP-1                                                          ST        831
      AREA=YSR(J)*ZS(K)                                                 ST        832
      ALX=RHO(LP)*U(LXP)*AREA                                           ST        833
      DIST=.5*XDIF(IS)                                                  ST        834
      IF (IS.EQ.2) DIST=XDIF(2)                                         ST        835
      TX=GAM(LP)*AREA/DIST                                              ST        836
      TX=AMAX1(TX,-ALX)                                                 ST        837
      CXU=ALX                                                           ST        838
      CX=TX+ALX                                                         ST        839
      TZFAC=R(J)/(R(M)+DFAC*(R(J)-R(M)))                                ST        840
      DO 72 I=IS,IE                                                     ST        841
      MAX=JWLO(I,NGOTO)-1                                               ST        842
      LIJ=JM(J)+I                                                       ST        843
      LP=KJM+I                                                          ST        844
      LXP=LP+1                                                          ST        845
      LYP=LP+NI                                                         ST        846
      LZP=LP+NINJ                                                       ST        847
      AXM(LIJ)=CX                                                       ST        848
      AYM(LIJ)=CY(I)                                                    ST        849
      AZM(LIJ)=CZ(LIJ)                                                  ST        850
      AREA=YSR(J)*ZS(K)                                                 ST        851
      IF (I.EQ.IF) GO TO 73                                             ST        852
      ALX=.25*(RHO(LP)+RHO(LXP))*U(LXP)*AREA                            ST        853
      TX=.5*(GAM(LP)+GAM(LXP))*AREA/XDIF(I+1)                           ST        854
      TX=AMAX1(TX,ABS(ALX))                                             ST        855
      CXUP=2.*ALX                                                       ST        856
      GO TO 74                                                          ST        857
   73 ALX=RHO(LXP)*U(LXP)*AREA                                          ST        858
      DIST=.5*XDIF(I+1)                                                 ST        859
      IF (I.EQ.L) DIST=XDIF(LP1)                                        ST        860
      TX=GAM(LXP)*AREA/DIST                                             ST        861
      TX=AMAX1(TX,ALX)                                                  ST        862
      CXUP=ALX                                                          ST        863
   74 AXP(LIJ)=TX-ALX                                                   ST        864
      CX=TX+ALX                                                         ST        865
      DIVG(LIJ)=DIVG(LIJ)+CXUP-CXU                                      ST        866
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      CXU=CXUP                                                          ST        867
      AREA=ZS(K)*XS(I)*RM(J+1)                                          ST        868
      IF (J.EQ.MAX) GO TO 75                                            ST        869
      ALY=.25*(RHO(LP)+RHO(LYP))*V(LYP)*AREA                            ST        870
      TY=.5*(GAM(LP)+GAM(LYP))*AREA/YDIF(J+1)                           ST        871
      TY=AMAX1(TY,ABS(ALY))                                             ST        872
      CYUP=2.*ALY                                                       ST        873
      GO TO 76                                                          ST        874
   75 ALY=RHO(LYP)*V(LYP)*AREA                                          ST        875
      DIST=.5*YDIF(J+1)                                                 ST        876
      IF (J.EQ.M) DIST=YDIF(MP1)                                        ST        877
      TY=GAM(LYP)*AREA/DIST                                             ST        878
      TY=AMAX1(TY,ALY)                                                  ST        879
      CYUP=ALY                                                          ST        880
   76 AYP(LIJ)=TY-ALY                                                   ST        881
      CY(I)=TY+ALY                                                      ST        882
      DIVG(LIJ)=DIVG(LIJ)+CYUP-CYU(I)                                   ST        883
      CYU(I)=CYUP                                                       ST        884
      AREA=XS(I)*YS(J)                                                  ST        885
      IF(K.EQ.N) GO TO 77                                               ST        886
      ALZ=.25*(RHO(LP)+RHO(LZP))*W(LZP)*AREA                            ST        887
      TZ=.5*(GAM(LP)+GAM(LZP))*AREA*TZFAC/(ZDIF(K+1)*R(J))              ST        888
      TZ=AMAX1(TZ,ABS(ALZ))                                             ST        889
      CZUP=2.*ALZ                                                       ST        890
      GO TO 78                                                          ST        891
   77 ALZ=RHO(LZP)*W(LZP)*AREA                                          ST        892
      ALZ=ALZ/2.                                                        ST        893
      TZ=GAM(LZP)*AREA*TZFAC/(ZSW(NP1)*R(J))                            ST        894
      TZ=AMAX1(TZ,ABS(ALZ))                                             ST        895
      CZUP=2.*ALZ                                                       ST        896
   78 AZP(LIJ)=TZ-ALZ                                                   ST        897
      CZ(LIJ)=TZ+ALZ                                                    ST        898
      DIVG(LIJ)=DIVG(LIJ)+CZUP-CZU(LIJ)                                 ST        899
      CZU(LIJ)=CZUP                                                     ST        900
      VOL=XS(I)*YSR(J)*ZS(K)                                            ST        901
79    ROT=0.                                                            ST        902
792   DIVG(LIJ)=AMAX1(ROT,DIVG(LIJ))                                   ST        903
      LPF=LP+NVM(NVF(NV))                                               ST        904
      SU(LIJ)=SU(LIJ)*VOL+DIVG(LIJ)*F(LPF)                              ST        905
      SP(LIJ)=SP(LIJ)*VOL-DIVG(LIJ)                                     ST        906
   72 CONTINUE                                                          ST        907
C-----SOURCE TERM MODIFICATIONS - BOUNDARY CONDITIONS.                  COMMENT   152
      CALL SOMOD                                                        ST        908
C-----CHEMICAL KINETICS CALCULATIONS.                                   COMMENT   153
C                                                                       COMMENT   154
      IF(NV.NE.LVH1)GO TO 722                                           NOX       230
      PA=PRESS                                                          NOX       231
      DO 723 J=2,M                                                      NOX       232
      IS=IMLI(J,NGOTO)                                                  NOX       233
      IE=IMLO(J,NGOTO)                                                  NOX       234
      DO 723 I=IS,IE                                                    NOX       235
      LIJ=I+JM(J)                                                       NOX       236
      LP=LIJ+KM(K)                                                      NOX       237
      TK=TEMP(LP)                                                       NOX       238
      ENV=AXP(LIJ)+AXM(LIJ)+AYP(LIJ)+AYM(LIJ)+AZP(LIJ)+AZM(LIJ)         NOX       239
C-----NODE IN BLOCKAGE - SKIP CALCULATION - GO TO 723                   COMMENT   155
      IF(ENV.LT.1.0E-10)GO TO 723                                       NOX       240
      ENV=ENV-SP(LIJ)                                                   NOX       241
      IF(ENV.GT.1.0E20)GO TO 723                                        NOX       242
      LPF=LP+1                                                          NOX       243
      LPM=LP-1                                                          NOX       244
      LPN=LP+NI                                                         NOX       245
      LPS=LP-NI                                                         NOX       246
      LPT=LP+NINJ                                                       NOX       247
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      LPW=LP-NTNJ                                                       NOX      248
      LIJ2=LIJ+KP(2)                                                    NOX      249
      LPFUOX=LP+NVM(NVFUOX)                                             NOX      250
      IF(ITR.NE.1)GO TO 741                                             NOX      251
      IF(ISTEP.NE.INOX)GO TO 741                                        NOX      252
C-----FIRST ITERATION - SET SPECIES CONCENTRATIONS EQUAL TO THOSE        COMMENT  156
C     AT NEIGHBORING NODE WHICH HAS ALREADY BEEN SOLVED.                COMMENT  157
      IF(IRES.NE.0)GO TO 741                                            JAN16      1
      IF(I.EQ.IS)GO TO 743                                              NOX      254
      DO 742 II=9,NS                                                    4STEP    329
      FS(LP,II)=FS(LPW,II)                                              NOX      256
      IF(I.NE.IE)FS(LPE,II)=FS(LPW,II)                                  NOX      257
      IF(J.NE.JWLO(I,NGOTO)-1)FS(LPN,II)=FS(LPW,II)                     NOX      258
      FS(LPT,II)=FS(LPW,II)                                             NOX      259
  742 IF(K.EQ.N)FS(LPT,II)=FS(LIJ2,II)                                  NOX      260
      GO TO 741                                                         NOX      261
  743 IF(J.EQ.JWLI(I,NGOTO)+1)GO TO 741                                 NOX      262
      DO 744 II=9,NS                                                    4STEP    330
      FS(LP,II)=FS(LPS,II)                                              NOX      264
      IF(I.NE.IE)FS(LPE,II)=FS(LPS,II)                                  NOX      265
      IF(J.NE.JWLO(I,NGOTO)-1)FS(LPN,II)=FS(LPS,II)                     NOX      266
      FS(LPT,II)=FS(LPS,II)                                             NOX      267
  744 IF(K.EQ.N)FS(LPT,II)=FS(LIJ2,II)                                  NOX      268
  741 CONTINUE                                                          NOX      269
C-----PREPARE INPUTS TO CHEMICAL KINETICS PROGRAM CREK.                 COMMENT  158
      DO 724 II=1,NS                                                    NOX      270
      S2(II)=FS(LP,II)/SMW(II)                                          NOX      271
  724 S1(II)=(AXP(LIJ)*FS(LPE,II)+AXM(LIJ)*FS(LPW,II)+AYP(LIJ)          NOX      272
     1*FS(LPN,II)+AYM(LIJ)*FS(LPS,II)+AZP(LIJ)*FS(LPT,II)+AZM(LIJ)      NOX      273
     2*FS(LPB,II))/(ENV*SMW(II))                                        NOX      274
      MSURO=F(LP+NVP(NVH))                                              NOX      275
      LPC=I-1+(J-2)*(NI-2)+(K-KSTR)*(NI-2)*(NJ-2)                       NOX      276
      EDKIJ=EDK(LPC)                                                    NOX      277
C-----NODEP=1, LAMINAR RATES USED.                                      COMMENT  159
      IF(NODER.EQ.1)EDKIJ=1.0E50                                        NOX      278
      FUT=F(LPFUOX)                                                     4STEP    331
      IF(NENZ.NE.0)S1(IDFU)=S1(IDFU)+EVAP(LPC)/(ENV*SMW(IDFU))          FEB2       3
      ENV=ENV/(XS(I)*YS*(J)*ZS(K))                                      NOX      280
      IF(TK.LT.TNOX)GO TO 735                                           NOX      281
C-----BYPASS CALCULATION IF TEMPERATURE.LT.TNOX (TNOX INPUT             COMMENT  160
C     BY USER).                                                         COMMENT  161
      CALL CREK                                                         NOX      282
C-----OUTPUTS FROM CREK.                                                COMMENT  162
      RHO(LP)=RHOPP                                                     NOX      283
      TEMP(LP)=TK                                                       NOX      284
C-----STORE SPECIES CONCENTRATONS IN RESPECTIVE ARRAYS.                 COMMENT  163
      DO 725 II=1,NS                                                    NOX      285
      FSLP=S2(II)*SMW(II)                                               NOX      286
      IF(FSLP.LT.1.0E-20)GO TO 725                                      NOX      287
C-----CHECK CONVERGENCE.                                                COMMENT  164
      IF(ABS(FSLP-FS(LP,II))/FSLP.GT.0.01)ICONVG=1                      NOX      288
  725 FS(LP,II)=FSLP                                                    NOX      289
      GO TO 738                                                         NOX      290
  735 CONTINUE                                                          NOX      291
      DO 736 II=9,NS                                                    4STEP    332
      FSLP=S1(II)*SMW(II)                                               NOX      293
      IF(FSLP.LT.1.0E-20)GO TO 736                                      NOX      294
      IF(ABS(FSLP-FS(LP,II))/FSLP.GT.0.01)ICONVG=1                      NOX      295
  736 FS(LP,II)=FSLP                                                    NOX      296
  738 CONTINUE                                                          NOX      297
      LPN2=LP+NVM(LVO2)                                                 NOX      298
      LPFU=LP+NVM(NVFU)                                                 NOX      299
      LPFU1=LP+NVM(LVFU1)                                               NOX      300
      LPCO=LP+NVM(NVCO)                                                 NOX      301
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      LPCO1=LP+NVM(LVCO1)                                                NOX      302
      F(LPFU1)=AMIN1(F(LPFU1),F(LPFUOK))                                 NOX      303
      F(LP02)=AMIN1(F(LP02),PATI02)                                      NOX      304
      F(LPFU)=F(LPFU1)                                                   NOX      305
      F(LPCO)=F(LPCO1)                                                   NOX      306
      LPCH=LP+NVM(NVCH)                                                  4STEP    333
      LPCH1=LP+NVM(LVCH1)                                                4STEP    334
      LPH2=LP+NVM(NVH2)                                                  4STEP    335
      LPH21=LP+NVM(LVH21)                                                4STEP    336
      F(LPCH)=F(LPCH1)                                                   4STEP    337
      F(LPH2)=F(LPH21)                                                   4STEP    338
  723 CONTINUE                                                           NOX      307
      GO TO 701                                                          NOX      308
C-----SOLVE FINITE-DIFFERENCE EQUATIONS IN SOLVE1 AND SOLVE2.            COMMENT  165
  727 CALL SOLVE1                                                        NOX      309
  701 CONTINUE                                                           ST       910
      IF(NV.NE.LVH1)CALL SOLVE2                                          NOX      310
      CALL FMOD                                                          ST       912
702   CONTINUE                                                           ST       913
      IF(ICONVG.EQ.0)GO TO 700                                           NOX      311
  706 CONTINUE                                                           NOX      312
  700 CONTINUE                                                           ST       914
C-----UPDATE DEPENDENT VARIABLE VALUES IN FMOD.                          COMMENT  166
      DO 705 INV=LVFU1,LVOH                                              NOX      313
      NV=INV                                                             NOX      314
  705 CALL FMOD                                                          NOX      315
      NV=LVFU1                                                           NOX      316
      CALL FMOD                                                          NOX      317
      NV=LVCO1                                                           NOX      318
      CALL FMOD                                                          NOX      319
      NV=LVFU                                                            NOX      320
      CALL FMOD                                                          NOX      321
      NV=LVCO                                                            NOX      322
      CALL FMCO                                                          NOX      323
      NV=LVCH                                                            4STEP    339
      CALL FMOD                                                          4STEP    340
      NV=LVH2                                                            4STEP    341
      CALL FMOD                                                          4STEP    342
      CALL DENMOD                                                        NOX      324
C-----OUTLET BOUNDARY.                                                   COMMENT  167
      DO 1005 J=1,MP1                                                    NOX      325
      DO 1005 K=2,N                                                      NOX      326
      LP=LP1+JM(J)+KM(K)                                                 NOX      327
 1005 TEMP(LP)=TEMP(LP-1)                                                NOX      328
      IF(IOW.NE.0)GO TO 1044                                             NOX      329
C-----SYMMETRY AXIS.                                                     COMMENT  168
      DO 1006 I=2,LP1                                                    NOX      330
      DO 1006 K=2,N                                                      NOX      331
      LP=I+KM(K)                                                         NOX      332
      LPN=LP+JM(2)                                                       NOX      333
 1006 TEMP(LP)=TEMP(LPN)                                                 NOX      334
C-----CYCLIC BOUNDARY CONDITIONS.                                        COMMENT  169
 1044 DO 1002 J=1,MP1                                                    NOX      335
      DO 1002 I=1,LP1                                                    NOX      336
      LIJ=I+JM(J)                                                        NOX      337
      LP2=I+JM(J)+KM(2)                                                  NOX      338
      LPN=LIJ+KM(N)                                                      NOX      339
      LPNP1=LIJ+KM(NP1)                                                  NOX      340
      TEMP(LIJ)=TEMP(LPN)                                                NOX      341
 1002 TEMP(LPNP1)=TEMP(LP2)                                              NOX      342
C +-+-+-+-+-+-+-+-+-+-+-+-+-+-   RADIATION EQUATIONS   +-+-+-+-+-+-+-+-+-+-+-+-+-+-  ST       915
C  ----- HERE U IS FX,  V IS FY,  W IS FZ                                ST       916
      READ (NTP1) U,V,W                                                  ST       917
      IND=0                                                              ST       918
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      DO 730 NV=LVRX,LVRZ                                                ST        919
      IF (ISOLVE(NV)) 733,730,733                                        ST        920
  733 IF (MOD(ISTEP,ISOLVE(NV))) 730,734,730                             ST        921
  734 IF (IND.EQ.0) CALL GAMRAD                                          ST        922
      IF (IPLAN.EQ.1) IND=1                                              ST        923
      CALL STRAD                                                         ST        924
      CALL FMOD                                                          ST        925
  730 CONTINUE                                                           ST        926
C  ----  COMPUTE AVG RADIATION FLUX  ------                             ST        927
      DO 740 K=1,NP1                                                     ST        928
      DO 740 J=1,NP1                                                     ST        929
      KJN=KN(K)+JN(J)                                                    ST        930
      DO 740 I=1,LP1                                                     ST        931
      LP=KJN+I                                                           ST        932
      LPRX=LP+NVP(NVRX)                                                  ST        933
      LPRY=LP+NVP(NVRY)                                                  ST        934
      LPRZ=LP+NVP(NVRZ)                                                  ST        935
      LPFAV=LP+NVP(NVFAV)                                                ST        936
  740 F(LPFAV)=(F(LPRX)+F(LPRY)+F(LPRZ))/3.                              ST        937
C -------- HERE PP IS PHI, P IS MFU, DU IS MCO                          ST        938
      WRITE (NTP2) PP,P,DU                                               ST        939
C -------- HERE DV IS ENTHALPY, DW IS FAV                               ST        940
      WRITE (NTP2) DV,DW                                                 ST        941
C  ------ HERE U IS FX,  V IS FY,  W IS FZ                              ST        942
      WRITE (NTP2) U,V,W                                                 ST        943
      WRITE (NTP2) TEMP,RHO                                              ST        944
      WRITE(NTP2)FCH,FH2                                                 4STEP     343
      WRITE(NTP2)ANUC,SOOT1,SOOT2                                        SOOT      403
      WRITE(NTP2)FS                                                      NOX       343
  799 NTPT=NTP1+NTP2                                                     ST        945
      NTP1=NTPT-NTP1                                                     ST        946
      NTP2=NTPT-NTP2                                                     ST        947
  800 ISTEP=ISTEP+1                                                      ST        948
      IXY= 3-IXY                                                         ST        949
      RETURN                                                             ST        950
      END                                                                ST        951
      SUBROUTINE STRAD                                                   STR         2
      COMMON/COEFF/A(40),B(40),EP(30),DP(30),APP(30),BPP(30)             NASAX      44
      COMMON F(35001),DU(500),DV(500),DW(500),                           COMFB       2
     1 ANUC(500),SOOT1(500),SOOT2(500),FCH(500),FH2(500),FS(500,14),     4STEP      18
     1 RHO(500),VISC(500),ABSR(500),SCTR(500),SU(100),SP(100),           RAD         3
     1 DRHODP(500),                                                      RAD         4
     1  AXP(100),AXM(100),AYP(100),AYM(100),AZP(100),                    COMFB       4
     2  AZM(100),CZ(100),CY(10),CZU(100),CYU(10),                        COMFB       5
     3  CZP(100),CYP(10),DIVG(100),NTP1,NTP2                             COMFB       6
     1,AXMK(192),AXPK(192),AYMK(192),AYPK(192),AZMK(192),AZPK(192),      CTDMA       3
     2 SUK(192),SPK(192)                                                 CTDMA       4
      DIMENSION U(500),V(500),W(500),PP(500),P(500),TEMP(500)            COMFB       7
      DIMENSION GAM(500)                                                 COMFB       8
      EQUIVALENCE (F(1),U(1)),(F(501),V(1)),(F(1001),W(1))               COMFB       9
      EQUIVALENCE (F(1501),PP(1)),(F(2001),P(1)),(F(2501),TEMP(1))       COMFB      10
      EQUIVALENCE (F(3001),GAM(1))                                       COMFB      11
      COMMON/CYL/R(30),RM(30),RMV(30),YSR(30),YSVR(30),IPLAN             COMMON      2
      COMMON/GRID/X(40),Y(30),Z(30),XS(40),YS(30),ZS(30),XSU(40),        COMMON      3
     1  YSV(30),ZSW(30),XDIF(40),YDIF(30),ZDIF(30),FXP(40),FXM(40),      COMMON      4
     2  FYP(30),FYM(30),FZP(30),FZM(30),DT,TIME                          COMMON      5
      COMMON                                                             NOX         2
     1/CINDEX/IDCO,IDFU,IDO2,IDN2,IDH2O,IDCO2,IDH1,IDH2,IDN1,IDNO,IDNO2  NOX         3
     1,IDO,IDOH,IMCPS,ILC,ILH,IMAT,ITER,JJJ,M1,M2,M3,MA,MGLOB,MGLOBP,    NOX         4
     2 NLM,NO,NSP,NS1,NS2,IDCH                                           4STEP       3
     3/CCHEMI/CPSUM,HSUM,FO,PPLN,RGAS,RGASIN,SMINV,TKINV,TLN,LNRG        NOX         6
     4/CPARAM/ASUB(30,3),ENV,ER,HSUBO,NDEBUG,NS,PA,QQ,Q1,Q2,Q3,Q4,RHOPP, NOX         7
     4 SM,SMW(30),SMO,S1(30),S2(30),TK,LADIAB,LDEBUG,LEQUIL,LREACT,      NOX         8
     4 LENER,EDKIJ,LCONVG                                                NOX         9
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      DOUBLE PRECISION CPSUM,ENV,ER,FQ,HSUBO,HSUM,PA,PPLN,Q0,Q1,Q2,Q3,    NOX      10
     1 Q4,RGAS,RGASIN,RHOPP,SM,SMINV,SMW,S1,S2,TK,TKINV,TLN,SMO           NOX      11
     2,FUT,FST                                                            4STEP     4
      COMMON/STEP4/PEXP1,PEXP2,PEXP3,PEXP4,ER1,ER2,ER3,ER4,CEBU1,CEBU2,   4STEP     5
     1 CEBU3,CEBU4,AEXP1,AEXP2,AEXP3,AEXP4,BEXP1,BEXP2,BEXP3,BEXP4,       4STEP     6
     2 CEXP1,CEXP2,CEXP3,CEXP4,FUT,FST                                    4STEP     7
      LOGICAL LADIAB,LCONVG,LDEBUG,LEQUIL,LNRG,LREACT,LENER               NOX      12
      COMMON/INT/L,M,N,LCV,MCV,NCV,LP1,MP1,NP1,NI,NJ,NK,NINJ,NINJNK,NV,   COMMON   6
     1 NNV,NGOTO,K,ISTR,JSTR,KSTR,NVM(35),KM(30),JM(30),ISTEP,            4STEP     8
     2 ISOLVE(32),IPRINT(33),TITLE(10,33),IXY,ISWP,JSWP,RELAX(35),MP,     4STEP     9
     3  NRHO,NGAM,IWLI(30,5),IWLO(30,5),JWLO(40,5),JWLI(40,5),IWEI,       COMMON    9
     4  IWEO,MM1,JWII,JWIO,JWO1,JWO0,IDM,JKIN(30,30),IKIN(40,30)          COMMON   10
      COMMON/INDEX/IPAR,LPREF,ISTUN,INCOMP,ITRAD,NVRX,NVRY,NVRZ,JPLANE    COMMON   11
     1,PLAKM1,LVK,LVD,LVFUOX,LVFU,LVCO,LVH,LVRX,LVRY,LVRZ,NVF(32),        4STEP    10
     2  IJUMP,IRES,TITLE2(20),IMAX,JMAX,KMAX,NVCO,FUNCC,NVH2O,NVCO2,      COMMON   13
     3 NVN2,NVCH,NVH2                                                     4STEP    11
      COMMON/CNOX/LVH1,LVH2,LVN1,LVNO,LVNO2,LVO,LVOH,LVH2O,LVN2,LVO2,     NOX      16
     1 LVCO2,LVFU1,LVCO1,NNOX,INOX,ITNOX,SNOX,TNOX                        NOX      17
      COMMON/THERM/NVH,NVFU,NVOX,NVFUOX,NVTE,NODEN,IDK,FSTOIC,HFU,CP,     COMMON   15
     1  GASCON,RHOCON,UNICON,PRESS,NVFAV,TCYLW,TINLW,TLIP,ACOEF(4),       COMMON   16
     2  T4,DFAC,WFU,WCO2,WCO,WOX,WH2O,WN2,HYY,CXX,RATIO1,RATIO2,          COMMON   17
     3  RATIO3,RATIO4,HCO,TAN,ITWALL                                      COMMON   18
      COMMON/CTDMA/KEND,ICTDMA(32)                                        4STEP    12
C-----SUBROUTINE STRAD IS USED FOR CALCULATING THE FINITE-                COMMENT  170
C     DIFFERENCE COEFFICIENTS IN THE RADIATION FLUX EQUATIONS             COMMENT  171
C     AND FOR SOLVING THESE EQUATIONS BY USING THE                        COMMENT  172
C     TRI-DIAGONAL-MATRIX-ALGORITHM(TDMA).                                COMMENT  173
C                                                                         COMMENT  174
      KONTRO=NV-LVRX+1                                                    STR      6
      GO TO (100,200,300),KONTRO                                          STR      7
C  -----   X-DIRECTION FLUX   ------                                       STR      8
  100 CONTINUE                                                            STR      9
      DO 101 K=2,N                                                        STR      10
      NVKM=NVM(NVRX)+KM(K)                                                STR      11
C-----OBTAIN SOURCE TERMS (SORAD) AND BOUNDARY CONDITIONS (SOMOD).        COMMENT  175
      CALL SORAD                                                          STR      12
      CALL SOMOD                                                          STR      13
      DO 102 J=2,M                                                        STR      14
      TX=0.                                                               STR      15
      IS=IWLI(J,NGOTO)                                                    STR      16
      IE=IWLO(J,NGOTO)                                                    STR      17
      DO 103 I=IS,IE                                                      STR      18
      LIJ=JM(J)+I                                                         STR      19
      LP=LIJ+KM(K)                                                        STR      20
      LXP=LP+1                                                            STR      21
      AXM(LIJ)=TX                                                         STR      22
      TX=.5*(GAM(LP)+GAM(LXP))/XDIF(I+1)                                  STR      23
      AXP(LIJ)=TX                                                         STR      24
      SU(LIJ)=SU(LIJ)*XS(I)                                               STR      25
      SP(LIJ)=SP(LIJ)*XS(I)                                               STR      26
  103 CONTINUE                                                            STR      27
      AXP(LIJ)=0.                                                         STR      28
  102 CONTINUE                                                            STR      29
C-----TDMA SOLUTION.                                                      COMMENT  176
      DO 104 J=2,M                                                        STR      30
      LPF=NVKM+JM(J)                                                      STR      31
      IS=IWLI(J,NGOTO)                                                    STR      32
      IE=IWLO(J,NGOTO)                                                    STR      33
      ISTR1=IS-1                                                          STR      34
      A(ISTR1)=0.                                                         STR      35
      B(ISTR1)=0.                                                         STR      36
      DO 105 I=IS,IE                                                      STR      37
      LIJ=JM(J)+I                                                         STR      38
      STORE=AYP(LIJ)+AYM(LIJ)-SP(LIJ)-AXM(LIJ)*A(I-1)                     STR      39
```

```
      A(I)=AXP(LIJ)/STORE                                                STR        40
  105 B(I)=(SU(LIJ)+AXM(LIJ)*B(I-1))/STORE                               STR        41
      ISUM=IS+IF                                                         STR        42
      DO 106 II=IS,IE                                                    STR        43
      I=ISUM-II                                                          STR        44
      LP=LPF+I                                                           STR        45
  106 F(LP)=A(I)*F(LP+1)+B(I)                                            STR        46
  104 CONTINUE                                                           STR        47
  101 CONTINUE                                                           STR        48
      RETURN                                                             STR        49
C  -----   Y-DIRECTION FLUX   ---                                        STR        50
  200 CONTINUE                                                           STR        51
      DO 201 K=2,N                                                       STR        52
      NVKM=NVP(NVRY)+KM(K)                                               STR        53
C-----OBTAIN SOURCE TERMS (SORAD) AND BOUNDARY CONDITIONS (SOMOD).       COMMENT    177
      CALL SORAD                                                         STR        54
      CALL SOMOD                                                         STR        55
      DO 202 I=2,L                                                       STR        56
      TY=0.                                                              STR        57
      JS=JWLI(I,NGOTO)+1                                                 STR        58
      JF=JWLO(I,NGOTO)-1                                                 STR        59
      DO 203 J=JS,JF                                                     STR        60
      LIJ=JP(J)+I                                                        STR        61
      LP=LIJ+KM(K)                                                       STR        62
      LYP=LP+NI                                                          STR        63
      AYM(LIJ)=TY                                                        STR        64
      TY=.5*(GAM(LP)+GAM(LYP))/YDIF(J+1)*RM(J+1)                         STR        65
      AYP(LIJ)=TY                                                        STR        66
      SU(LIJ)=SU(LIJ)*YS(J)*R(J)                                         STR        67
      SP(LIJ)=SP(LIJ)*YS(J)*R(J)                                         STR        68
  203 CONTINUE                                                           STR        69
      AYP(LIJ)=0.                                                        STR        70
  202 CONTINUE                                                           STR        71
C-----TDMA SOLUTION.                                                     COMMENT    178
      DO 204 I=2,L                                                       STR        72
      LPF=NVKM+I                                                         STR        73
      JS=JWLI(I,NGOTO)+1                                                 STR        74
      JF=JWLO(I,NGOTO)-1                                                 STR        75
      JSTR1=JS-1                                                         STR        76
      A(JSTR1)=0.                                                        STR        77
      B(JSTR1)=0.                                                        STR        78
      DO 205 J=JS,JE                                                     STR        79
      LIJ=JM(J)+I                                                        STR        80
      STORE=AYP(LIJ)+AYM(LIJ)-SP(LIJ)-AYM(LIJ)*A(J-1)                    STR        81
      A(J)=AYP(LIJ)/STORE                                                STR        82
  205 B(J)=(SU(LIJ)+AYM(LIJ)*B(J-1))/STORE                               STR        83
      JSUM=JS+JE                                                         STR        84
      DO 206 JJ=JS,JE                                                    STR        85
      J=JSUM-JJ                                                          STR        86
      LP=LPF+JR(J)                                                       STR        87
      LYP=LP+NI                                                          STR        88
  206 F(LP)=A(J)*F(LYP)+B(J)                                             STR        89
  204 CONTINUE                                                           STR        90
  201 CONTINUE                                                           STR        91
      RETURN                                                             STR        92
C  -----   Z-DIRECTION FLUX   ---                                        STR        93
  300 KSUM=2+N                                                           STR        94
      DO 301 J=2,M                                                       STR        95
      JPLANE=J                                                           STR        96
      NVJM=NVP(NVRZ)+JM(J)                                               STR        97
C-----OBTAIN SOURCE TERMS (SORAD) AND BOUNDARY CONDITIONS (SOMODZ).      COMMENT    179
      CALL SORAD                                                         STR        98
      CALL SOMODZ                                                        STR        99
      IS=IWLI(J,NGOTO)                                                   STR       100
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      IF=IWLO(J,NGOTO)                                                  STR     101
      DO 302 I=IS,IF                                                    STR     102
      LIJ=JM(J)+I                                                       STR     103
      TZ=0.                                                             STR     104
      DO 303 K=2,N                                                      STR     105
      LIK=JM(K)+I                                                       STR     106
      LP=LIJ+KM(K)                                                      STR     107
      LZP=LP+NINJ                                                       STR     108
      AZM(LIK)=TZ                                                       STR     109
      TZ=.5*(GAM(LP)+GAM(LZP))/(ZDIF(K+1)*R(J))                         STR     110
      AZP(LIK)=TZ                                                       STR     111
      SU(LIK)=SU(LIK)*ZS(K)*R(J)                                        STR     112
      SP(LIK)=SP(LIK)*ZS(K)*R(J)                                        STR     113
  303 CONTINUE                                                          STR     114
      AZP(LIK)=0.                                                       STR     115
  302 CONTINUE                                                          STR     116
C-----TOMA SOLUTION.                                                    COMMENT 180
      DO 304 I=IS,IE                                                    STR     117
      A(1)=0.                                                           STR     118
      B(1)=0.                                                           STR     119
      LPF=NVJM+I                                                        STR     120
      DO 305 K=2,N                                                      STR     121
      LIK=JM(K)+I                                                       STR     122
      STORE=AZP(LIK)+AZM(LIK)-SP(LIK)-AZM(LIK)*A(K-1)                   STR     123
      A(K)=AZP(LIK)/STORE                                               STR     124
  305 B(K)=(SU(LIK)+AZM(LIK)*B(K-1))/STORE                              STR     125
      DO 306 KK=2,N                                                     STR     126
      K=KSUM-KK                                                         STR     127
      LP=LPF+KM(K)                                                      STR     128
      LZP=LP+NINJ                                                       STR     129
  306 F(LP)=A(K)*F(LZP)+B(K)                                            STR     130
  304 CONTINUE                                                          STR     131
  301 CONTINUE                                                          STR     132
      RETURN                                                            STR     133
      END                                                               STR     134
      FUNCTION TSOLVE(TWN,TGAS,RAD,HTCI,STG,EMI,ITRAD)                  TSO       2
C-----SOLVE FOR WALL TEMPERATURES.                                      COMMENT 181
      ITR=MIND(ITRAD,2)                                                 TSO       3
      KOUNT=0                                                           TSO       4
   10 TW=TWN                                                            TSO       5
      KOUNT=KOUNT+1                                                     TSO       6
      IF(KOUNT.GT.10)GO TO 30                                           TSO       7
      TW2=TW*TW                                                         TSO       8
C-----RADIATION.                                                        COMMENT 182
      QRH=2.0*EMI*(STG*TW2*TW2-RAD)*FLOAT(ITR-1)                        TSO       9
C-----CONVECTION.                                                       COMMENT 183
      QCH=HTCI*(TW-TGAS)                                                TSO      10
      DQRH=8.0*EMI*STG*TW*TW2*FLOAT(ITR-1)                              TSO      11
      DQCH=HTCI                                                         TSO      12
      FTW=QRH+QCH                                                       TSO      13
      DFTW=DQRH+DQCH                                                    TSO      14
      TWN=TW-FTW/(DFTW+1.E-30)                                          TSO      15
      IF(ABS(TWN/TW-1.).GT..001)GO TO 10                                TSO      16
   30 TSOLVE=TWN                                                        TSO      17
      RETURN                                                            TSO      18
      END                                                               TSO      19
      SUBROUTINE ABSORB(TS,T,PATH,SQOTK,PCO2,PH2O,ALPHA)                ABSOR     2
C                                                                       ABSOR     3
C                                                                       ABSOR     4
C                                                                       ABSOR     5
C        SUBROUTINE ABSROB COMPUTES THE ABSORPTIVITIES (WITH RESPECT TO ABSOR     6
C        A BLACKBODY SOURCE) OF ISOTHERMAL , HOMOGENEOUS MIXTURES OF SOO ABSOR     7
C        CO2 AND H2O AT A TOTAL PRESSURE OF 1 ATMOSPHERE.  ABSORPTIVITIE ABSOR     8
C        CALCULATED BY SUBROUTINE ABSORB ARE IN GOOD AGREEMENT WITH       ABSOR     9
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C     EXPERIMENTAL MEASUREMENTS.                                        ABSOR   10
C                                                                       ABSOR   11
C                                                                       ABSOR   12
C                                                                       ABSOR   13
C     FOR A BLACKBODY SOURCE TEMPERATURE EQUAL TO THE MIXTURE           ABSOR   14
C     TEMPERATURE, ABSORPTIVITY EQUALS EMISSIVITY.  EMISSIVITIES SO     ABSOR   15
C     CALCULATED ARE IN GOOD AGREEMENT WITH SPECTRAL CALCULATIONS       ABSOR   16
C     AND WITH EXPERIMENTAL MEASUREMENTS.                               ABSOR   17
C                                                                       ABSOR   18
C                                                                       ABSOR   19
C                                                                       ABSOR   20
C     EACH CALL ON SUBROUTINE ABSORB REQUIRES LESS THAN 12 MILLISECON   ABSOR   21
C     OF CPU TIME ON AN IBM 370/158.                                    ABSOR   22
C                                                                       ABSOR   23
C                                                                       ABSOR   24
C                                                                       ABSOR   25
C     INPUTS:                                                           ABSOR   26
C                                                                       ABSOR   27
C                                                                       ABSOR   28
C     1. TS (IN DEGREES KELVIN):  BLACKBODY SOURCE TEMPERATURE.         ABSOR   29
C     TS MUST BE GREATER THAN OR EQUAL TO 300.K AND LESS THAN OR        ABSOR   30
C     EQUAL TO 2000.K.                                                  ABSOR   31
C                                                                       ABSOR   32
C                                                                       ABSOR   33
C     2. T (IN DEGREES KELVIN):  MIXTURE TEMPERATURE.  T MUST BE GREAT  ABSOR   34
C     THAN OR EQUAL TO 300.K AND LESS THAN OR EQUAL TO 2000.K.          ABSOR   35
C                                                                       ABSOR   36
C                                                                       ABSOR   37
C     3. PATH (IN METRES):  MIXTURE PATHLENGTH.  PATH MUST BE           ABSOR   38
C     GREATER THAN OR EQUAL TO 0.0 METRES.                              ABSOR   39
C                                                                       ABSOR   40
C                                                                       ABSOR   41
C     4. SOOTK (IN INVERSE METRES):  ABSORPTION COEFFICIENT OF SOOT     ABSOR   42
C     AT A WAVELENGTH OF 0.94 MICROMETRES.  SOOTK IS (APPROXIMATELY)    ABSOR   43
C     RELATED TO THE SOOT VOLUME FRACTION, FV, BY:SOOTK=7FV/0.94E-6.    ABSOR   44
C     SOOTK MUST BE GREATER THAN OR EQUAL TO 0.0 INVERSE METRES.        ABSOR   45
C                                                                       ABSOR   46
C                                                                       ABSOR   47
C     5. PCO2 (IN ATMOSPHERES):  PARTIAL PRESSURE OF CO2 IN A MIXTURE   ABSOR   48
C     WHOSE TOTAL PRESSURE IS 1 ATMOSPHERE.  PCO2 MUST BE GREATER       ABSOR   49
C     THAN OR EQUAL TO 0.0 ATMOSPHERES AND LESS THAN OR EQUAL  TO       ABSOR   50
C     1.0 ATMOSPHERES.  FOR PCO2 LESS THAN 0.0011 ATMOSPHERES, THE      ABSOR   51
C     CONTRIBUTION OF CO2 TO THE MIXTURE ABSORPTIVITY IS ASSUMED TO     ABSOR   52
C     BE ZERO.  FOR (PATH*TS/T*PCO2) LESS THAN 0.0011 ATM-METRE, THE    ABSOR   53
C     CONTRIBUTION OF CO2 TO THE MIXTURE ABSORPTIVITY IS ASSUMED TO     ABSOR   54
C     BE ZERO.  IF (PATH*TS/T*PCO2) EXCEEDS 9.98 ATM-METRE,            ABSOR   55
C     SUBROUTINE ABSORB ABORTS AND RETURNS A VALUE OF ABSORPTIVITY      ABSOR   56
C     SET AT -1.E30.  A DIAGNOSTIC MESSAGE IS PROVIDED.                 ABSOR   57
C                                                                       ABSOR   58
C                                                                       ABSOR   59
C     6. PH2O (IN ATMOSPHERES):  PARTIAL PRESSURE OF H2O IN A MIXTURE   ABSOR   60
C     WHOSE TOTAL PRESSURE IS 1 ATMOSPHERE.  PH2O MUST BE GREATER       ABSOR   61
C     THAN OR EQUAL TO 0.0 ATM AND LESS THAN OR EQUAL TO (1.0-PCO2) A   ABSOR   62
C     FOR PH2O LESS THAN 0.0011 ATM, THE CONTRIBUTION OF H2O TO THE     ABSOR   63
C     MIXTURE ABSORPTIVITY IS ASSUMED TO BE ZERO.  FOR (PATH*TS/T*PH2   ABSOR   64
C     LESS THAN 0.0011 ATM-METRE, THE CONTRIBUTION OF H2O TO THE        ABSOR   65
C     MIXTURE ABSORPTIVITY IS ASSUMED TO BE ZERO.  IF (PATH*TS/T*PH2O   ABSOR   66
C     EXCEEDS 9.98 ATM-METRE, SUBROUTINE ABSORB ABORTS AND RETURNS A    ABSOR   67
C     VALUE OF ABSORPTIVITY SET AT -1.E30.  A DIAGNOSTIC MESSAGE        ABSOR   68
C     IS PROVIDED.                                                      ABSOR   69
C                                                                       ABSOR   70
C                                                                       ABSOR   71
C                                                                       ABSOR   72
C     OUTPUT:                                                           ABSOR   73
```

```
C
C
C         SUBROUTINE ABSORB RETURNS ALPHA   THE (DIMENSIONLESS)
C         ABSORPTIVITY OF A MIXTURE OF SOOT, CO2 AND H2O AT A TOTAL
C         PRESSURE OF 1 ATMOSPHERE.
C
C
C         THE FOLLOWING SUBROUTINES MUST BE USED WITH
C         ABSORBG
C         1. ASYMP
C         2. CHEBY
C         3. DLECK
C         4. FGAS
C         5. PENTA
C         6. SOOT
C         7. SCRTCH
C
C
C
C         QUESTIONS ABOUT SUBROUTINE ABSORB MAY BE ADDRESSED TO:
C         ASHOK T. MODAK
C         NORTHERN RESEARCH AND ENGINEERING CORPORATION
C         WOBURN, MASS. 01801
C         USA
C         TEL. NO. (617) 935-9050 EXT 264.
C
C
C
      IF(TS.LT.300.     .OR.     TS.GT.2000.)GOTO 1
      IF(T .LT.300.     .OR.     T .GT.2000.)GOTO 2
      PSUM=PCO2+PH2O
      IF(PSUM.GT.1.0)  GOTO 3
C COMPUTE RATIO OF MIXTURE AND SOURCE TEMPERATURES.
      RATIO=T/TS
C COMPUTE EFFECTIVE PATHLENGTH,PATHL
      PATHL=PATH/RATIO
      PCL=PCO2*PATHL
      PWL=PH2O*PATHL
      IF(PCL.GT.5.98     .OR.     PWL.GT.5.98)  GOTO 4
C COMPUTE SOOT ABSORPTIVITY,AS
      AS=0.0
      IF(SOOTK.LE.0.0)  GOTO 51
      CALL SOOT(SOOTK,PATH,TS,TAUS)
      AS=1.-TAUS
C
C
   51 CONTINUE
C COMPUTE GAS ABSORPTIVITY,AG
      AG=0.0
      IF(PCO2.LT.0.0011     .AND.     PH2O.LT.0.0011)GOTO 52
      IF(PCL .LT.0.0011     .AND.     PWL .LT.0.0011)GOTO 52
      AG=FGAS(PATHL,PCO2,PH2O,TS)
C COMPUTE WATER VAPOR FRACTION,ZETA
      ZETA=PH2O/PSUM
      POWER=0.65-0.2*ZETA
      AG=AG*RATIO**POWER
   52 CONTINUE
      ALPHA=AS+AG-AS*AG
      RETURN
    4 CONTINUE
      WRITE(6,5)
    5 FORMAT(' EITHER THE PRODUCT,PATH.TS/T.PCO2,OR PATH.TS/T.PH2O EXCEE
     1DS 5.98 ATM-METRES')
      WRITE(6,6)
```


ORIGINAL PAGE IS
OF POOR QUALITY

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    6 FORMAT(* THIS CALCULATION LIES OUTSIDE THE RANGE OF SUBROUTINE ABS ABSOR  138
     1ORB.SUBROUTINE ABSORB ABORTS AND RETURNS A VALUE OF*)              ABSOR  139
       WRITE(6,7)                                                       ABSOR  140
     7 FORMAT(* ALPHA SET EQUAL TO -1.E30*)                             ABSOR  141
       GOTO 8                                                           ABSOR  142
     3 CONTINUE                                                         ABSOR  143
       WRITE(6,9)                                                       ABSOR  144
     9 FORMAT(* SUM OF GAS PARTIAL PRESSURES,PCO2+PH2O,EXCEEDS 1 ATM*)  ABSOR  145
       WRITE(6,6)                                                       ABSOR  146
       WRITE(6,7)                                                       ABSOR  147
       GOTO 8                                                           ABSOR  148
     2 CONTINUE                                                         ABSOR  149
       WRITE(6,11)                                                      ABSOR  150
    11 FORMAT(* MIXTURE TEMPERATURE ,T, LIES OUTSIDE THE TEMPERATURE RANG ABSOR  151
      1E 300 TO 2000 DEGREES KELVIN*)                                   ABSOR  152
       WRITE(6,6)                                                       ABSOR  153
       WRITE(6,7)                                                       ABSOR  154
       GOTO 8                                                           ABSOR  155
     1 CONTINUE                                                         ABSOR  156
       WRITE(6,10)                                                      ABSOR  157
    10 FORMAT(* BLACKBODY SOURCE TEMPERATURE,TS,LIES OUTSIDE THE TEMPERAT ABSOR  158
      1URE RANGE 300 TO 2000 DEGREES KELVIN*)                           ABSOR  159
       WRITE(6,6)                                                       ABSOR  160
       WRITE(6,7)                                                       ABSOR  161
     8 CONTINUE                                                         ABSOR  162
       ALPHA=-1.E30                                                     ABSOR  163
       RETURN                                                           ABSOR  164
       END                                                              ABSOR  165
       SUBROUTINE ASYMP(Z,ZV)                                           ABSOR  166
C         SUBROUTINE ASYMP COMPUTES THE ASYMPTOTIC EXPANSION FOR THE     ABSOR  167
C         PENTAGAMMA FUNCTION.                                           ABSOR  168
C                                                                        ABSOR  169
       ZI1=1./Z                                                         ABSOR  170
       ZI2=ZI1*ZI1                                                      ABSOR  171
       ZI3=ZI1*ZI2                                                      ABSOR  172
       ZV=ZI3*((2.+3.*ZI1)+ZI2*(2.+ZI2*(-1.+ZI2*(1.333333333           ABSOR  173
      1  +ZI2*(-3.+10.*ZI2)))))                                         ABSOR  174
       RETURN                                                           ABSOR  175
       END                                                              ABSOR  176
       SUBROUTINE CHEBY(N,X,V)                                          ABSOR  177
C         V REPRESENTS VALUE OF CHEBYSHEV POLYNOMIAL OF ORDER N        ABSOR  178
C         AND ARGUMENT X.                                              ABSOR  179
       V=1.                                                             ABSOR  180
       IF(N)  1,1,2                                                     ABSOR  181
     1 RETURN                                                           ABSOR  182
C                                                                       ABSOR  183
     2 V=X                                                              ABSOR  184
       IF(N-1)  1,1,3                                                   ABSOR  185
     3 F=2.*X                                                           ABSOR  186
       VM1=X                                                            ABSOR  187
       VM2=1.                                                           ABSOR  188
       DO 4 I=2,N                                                       ABSOR  189
       V=F*VM1-VM2                                                      ABSOR  190
       VM2=VM1                                                          ABSOR  191
       VM1=V                                                            ABSOR  192
     4 CONTINUE                                                         ABSOR  193
       RETURN                                                           ABSOR  194
       END                                                              ABSOR  195
       FUNCTION OLECK(X,PL,T)                                           ABSOR  196
C         SUBROUTINE OLECK COMPUTES THE 2.7 AND 15 MICRONSTRE OVERLAP    ABSOR  197
C         CORRECTION FOR MIXTURES OF CO2 AND H2O.  THE OVERLAP CORRECTION ABSOR  198
C         IS COMPUTED BY USING A TEMPERATURE-ADJUSTED VERSION OF THE     ABSOR  199
C         OVERLAP CORRECTION FACTOR SUGGESTED BY R. LECKNER              ABSOR  200
C         (COMBUSTION AND FLAME VOLUME 19 PAGES 33-48, 1972)             ABSOR  201
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      IF(PL.LT.0.1)   GOTO 1                                                ABSOR   202
      TERM=X/(10.7+101.*X)  -X**10.4/111.7                                  ABSOR   203
      TERM2=ALOG10(101.325*PL)                                              ABSOR   204
      TERM2=TERM2**2.76                                                     ABSOR   205
      TT=T/1000.                                                            ABSOR   206
      TT2=TT*TT                                                             ABSOR   207
      A=-1.0204082                                                          ABSOR   208
      B=2.2448979                                                           ABSOR   209
      C=-0.22449306                                                         ABSOR   210
      TERM3=A*TT2+  B*TT  +  C                                              ABSOR   211
C        TERM3 REPRESENTS THE TEMPERATURE ADJUSTMENT                        ABSOR   212
      DLECK=TERM *TERM2*TERM3                                               ABSOR   213
      RETURN                                                                ABSOR   214
    1 DLECK=0.0                                                             ABSOR   215
      RETURN                                                                ABSOR   216
      END                                                                   ABSOR   217
      FUNCTION EGAS(PATHL,PC,PW,T)                                          ABSOR   218
C        FUNCTION EGAS COMPUTES THE EMISSIVITY OF A GIVEN PATH (PATHL)      ABSOR   219
C        OF A MIXTURE OF CO2 AND H2O AT TEMPERATURE T.                      ABSOR   220
C                                                                           ABSOR   221
C        PC - PARTIAL PRESSURE OF CO2                                       ABSOR   222
C        PW - PARTIAL PRESSURE OF H2O                                       ABSOR   223
      EGAS=0.0                                                              ABSOR   224
      IF(T.LT.300.  .OR.  T.GT.2000.) RETURN                                ABSOR   225
      EC=0.0                                                                ABSOR   226
      IF(PC.LT.0.0011  .OR.  PC.GT.1.0)  GOTO 1                             ABSOR   227
      PCL=PC*PATHL                                                          ABSOR   228
      IF(PCL.LT.0.0011  .OR.  PCL.GT.5.98)  GOTO 1                          ABSOR   229
      CALL SCRTCH(PC,PCL,T,1,EC)                                            ABSOR   230
    1 CONTINUE                                                              ABSOR   231
      IF(PW.LT.0.0011  .OR.  PW.GT.1.0)  GOTO 2                             ABSOR   232
      PWL=PW*PATHL                                                          ABSOR   233
      IF(PWL.LT.0.0011  .OR.  PWL.GT.5.98)  GOTO 2                          ABSOR   234
      CALL SCRTCH(PW,PWL,T,2,EW)                                            ABSOR   235
      EGAS=EC+EW                                                            ABSOR   236
      IF(EC.LE.C.0)  RETURN                                                 ABSOR   237
      PCPW=PC+PW                                                            ABSOR   238
      XI=PW/PCPW                                                            ABSOR   239
      IF(XI.LT.0.01)  RETURN                                                ABSOR   240
      PCWL=PCPW*PATHL                                                       ABSOR   241
      IF(PCWL.LT.0.1   ) RETURN                                             ABSOR   242
      DELE=DLECK(XI,PCWL,T)                                                 ABSOR   243
      EGAS=EGAS-DELE                                                        ABSOR   244
      RETURN                                                                ABSOR   245
    2 CONTINUE                                                              ABSOR   246
      EGAS=EC                                                               ABSOR   247
      RETURN                                                                ABSOR   248
      END                                                                   ABSOR   249
      SUBROUTINE PENTA(X,V)                                                 ABSOR   250
C        SUBROUTINE PENTA RETURNS THE VALUE V OF THE PENTAGAMMA FUNCTION    ABSOR   251
C        OF ARGUMENT X.  RECURRENCE FORMULA 6.4.6, AND ASYMPTOTIC FORMUL    ABSOR   252
C        6.4.14 (PAGE 260) OF ABRAMOWITZ AND STEGUN ARE USED IN             ABSOR   253
C        THIS CALCULATION.                                                  ABSOR   254
C                                                                           ABSOR   255
C                                                                           ABSOR   256
C                                                                           ABSOR   257
      IF(X.GE.4.)  GOTO 1                                                   ABSOR   258
      IF(X.GE.3.)  GOTO 2                                                   ABSOR   259
      IF(X.GE.2.)  GOTO 3                                                   ABSOR   260
      S=(1./(X+2.)**4+1./(X+1.)**4+1./X**4)*6.                              ABSOR   261
      Z=X+3.                                                                ABSOR   262
      CALL ASYMP(Z,ZV)                                                      ABSOR   263
      GOTO 4                                                                ABSOR   264
    3 CONTINUE                                                              ABSOR   265
      S=(1./(X+1.)**4+1./X**4)*6.
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      Z=X+2.                                                            ABSOR   266
      CALL ASYMP(Z,ZV)                                                  ABSOR   267
      GOTO 4                                                            ABSOR   268
    2 CONTINUE                                                          ABSOR   269
      S=6./X**4                                                         ABSOR   270
      Z=X+1.                                                            ABSOR   271
      CALL ASYMP(Z,ZV)                                                  ABSOR   272
      GOTO 4                                                            ABSOR   273
    1 CONTINUE                                                          ABSOR   274
      S=0.0                                                             ABSOR   275
      CALL ASYMP(X,ZV)                                                  ABSOR   276
    4 CONTINUE                                                          ABSOR   277
      V=ZV+S                                                            ABSOR   278
      RETURN                                                            ABSOR   279
      END                                                               ABSOR   280
      SUBROUTINE SOOT(ZKLED,PATHL,TBLACK,TAUS)                          ABSOR   281
C        SUBROUTINE SOOT COMPUTES THE TRANSMISSIVITY (TAUS) OF PATH (PAT ABSOR   282
C        OF SOOT TO A BLACKBODY RADIATION SOURCE AT A GIVEN              ABSOR   283
C        TEMPERATURE (TBLACK).                                          ABSOR   284
C                                                                        ABSOR   285
      IF(ZKLED.LE. 0.)  GOTO 1                                          ABSOR   286
      ARG=1.+ZKLED*PATHL*TBLACK*6.5337E-5                               ABSOR   287
C        TBLACK - SOURCE TEMPERATURE OR GAS TEMPERATURE                  ABSOR   288
      CALL PENTA(ARG,V)                                                 ABSOR   289
C        SUBROUTINE PENTA COMPUTES THE PENTAGAMMA FUNCTION               ABSOR   290
C        ARG - ARGUMENT  OF THE PENTAGAMMA FUNCTION                      ABSOR   291
      TAUS=V*.1539897336                                                ABSOR   292
C        TAUS - SOOT TRANSMISSIVITY                                      ABSOR   293
      RETURN                                                            ABSOR   294
    1 TAUS=1.                                                           ABSOR   295
      RETURN                                                            ABSOR   296
      END                                                               ABSOR   297
      SUBROUTINE SCRTCH(P,PL,T,INDEX,V)                                 ABSOR   298
      DIMENSION CC(3,4,4),CW(3,4,4),          SC(3,4,4)                 ABSOR   299
      IF(INDEX.EQ.2)  GOTO 2                                            ABSOR   300
C        CC REPRESENTS AN ARRAY OF 48 COEFFICIENTS FOR CO2               ABSOR   301
C                                                                        ABSOR   302
C                                                                        ABSOR   303
C                                                                        ABSOR   304
      CC(1,1,1)=-0.2754568E+01                                          ABSOR   305
      CC(1,1,2)=-0.2997857E+00                                          ABSOR   306
      CC(1,1,3)=-0.1232494E+00                                          ABSOR   307
      CC(1,1,4)=0.1279287E-01                                           ABSOR   308
      CC(1,2,1)=0.1503051E+01                                           ABSOR   309
      CC(1,2,2)=0.3156449E+00                                           ABSOR   310
      CC(1,2,3)=0.1058126E-01                                           ABSOR   311
      CC(1,2,4)=-0.3729625E-01                                          ABSOR   312
      CC(1,3,1)=-0.2474119E+00                                          ABSOR   313
      CC(1,3,2)=-0.3323046E-01                                          ABSOR   314
      CC(1,3,3)=-0.1819471E-01                                          ABSOR   315
      CC(1,3,4)=0.2289709E-01                                           ABSOR   316
      CC(1,4,1)=0.4994029E-01                                           ABSOR   317
      CC(1,4,2)=-0.1986786E-02                                          ABSOR   318
      CC(1,4,3)=0.3007898E-02                                           ABSOR   319
      CC(1,4,4)=-0.1179598E-02                                          ABSOR   320
      CC(2,1,1)=0.5737722E-02                                           ABSOR   321
      CC(2,1,2)=-0.9328458E-02                                          ABSOR   322
      CC(2,1,3)=0.2906266E-02                                           ABSOR   323
      CC(2,1,4)=0.4227520E-03                                           ABSOR   324
      CC(2,2,1)=-0.3151784E-02                                          ABSOR   325
      CC(2,2,2)=0.5832821E-02                                           ABSOR   326
      CC(2,2,3)=-0.3260295E-02                                          ABSOR   327
      CC(2,2,4)=0.7065884E-03                                           ABSOR   328
      CC(2,3,1)=0.1668751E-03                                           ABSOR   329
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      CC(2,3,2)=-0.7326533E-03                                          ABSOR  330
      CC(2,3,3)=0.3639855E-03                                           ABSOR  331
      CC(2,3,4)=0.3220318E-03                                           ABSOR  332
      CC(2,4,1)=0.7306638E-03                                           ABSOR  333
      CC(2,4,2)=-0.7277073E-03                                          ABSOR  334
      CC(2,4,3)=0.5925968E-03                                           ABSOR  335
      CC(2,4,4)=-0.2021413E-03                                          ABSOR  336
      CC(3,1,1)=0.3365611E-02                                           ABSOR  337
      CC(3,1,2)=-0.9439185E-02                                          ABSOR  338
      CC(3,1,3)=0.1764560E-02                                           ABSOR  339
      CC(3,1,4)=0.3C35031E-03                                           ABSOR  340
      CC(3,2,1)=-0.1062700E-02                                          ABSOR  341
      CC(3,2,2)=0.9236759E-02                                           ABSOR  342
      CC(3,2,3)=-C.1952250E-02                                          ABSOR  343
      CC(3,2,4)=0.3474022E-03                                           ABSOR  344
      CC(3,3,1)=0.1204807E-03                                           ABSOR  345
      CC(3,3,2)=-0.4479927E-03                                          ABSOR  346
      CC(3,3,3)=0.2497521E-03                                           ABSOR  347
      CC(3,3,4)=0.1812996E-03                                           ABSOR  348
      CC(3,4,1)=0.4218169E-03                                           ABSOR  349
      CC(3,4,2)=-0.4046608E-03                                          A  R   350
      CC(3,4,3)=0.3256861E-03                                           ABSOR  351
      CC(3,4,4)=-0.9514981E-04                                          ABSOR  352
      GOTO4                                                             ABSOR  353
    2 CONTINUE                                                          ABSOR  354
C         CW REPRESENTS AN ARRAY OF 48 COEFFICIENTS FOR H2O             ABSOR  355
C                                                                       ABSOR  356
C                                                                       ABSOR  357
      CW(1,1,1)=-0.2594279E+01                                          ABSOR  358
      CW(1,1,2)=-0.7118472E+00                                          ABSOR  359
      CW(1,1,3)=-0.9956839E-03                                          ABSOR  360
      CW(1,1,4)=0.1226960E-01                                           ABSOR  361
      CW(1,2,1)=0.2510331E+01                                           ABSOR  362
      CW(1,2,2)=0.6481808E+00                                           ABSOR  363
      CW(1,2,3)=-0.3330597E-01                                          ABSOR  364
      CW(1,2,4)=-0.5524345E-02                                          ABSOR  365
      CW(1,3,1)=-0.4191636E+00                                          ABSOR  366
      CW(1,3,2)=-0.1375180E+00                                          ABSOR  367
      CW(1,3,3)=0.3877930E-01                                           ABSOR  368
      CW(1,3,4)=0.8862328E-03                                           ABSOR  369
      CW(1,4,1)=-0.3223912E-01                                          ABSOR  370
      CW(1,4,2)=-0.1020241E-01                                          ABSOR  371
      CW(1,4,3)=-0.2223143E-01                                          ABSOR  372
      CW(1,4,4)=-0.5940781E-03                                          ABSOR  373
      CW(2,1,1)=0.1126969E+00                                           ABSOR  374
      CW(2,1,2)=-C.8133829E-01                                          ABSOR  375
      CW(2,1,3)=0.1514940E-01                                           ABSOR  376
      CW(2,1,4)=0.1393880E-02                                           ABSOR  377
      CW(2,2,1)=-C.9298805E-02                                          ABSOR  378
      CW(2,2,2)=0.4550660E-01                                           ABSOR  379
      CW(2,2,3)=-C.2082009E-01                                          ABSOR  380
      CW(2,2,4)=0.2013961E-02                                           ABSOR  381
      CW(2,3,1)=-C.4375032E-01                                          ABSOR  382
      CW(2,3,2)=0.1924597E-01                                           ABSOR  383
      CW(2,3,3)=0.8859877E-02                                           ABSOR  384
      CW(2,3,4)=-0.4618414E-02                                          ABSOR  385
      CW(2,4,1)=0.7077876E-02                                           ABSOR  386
      CW(2,4,2)=-C.2096188E-01                                          ABSOR  387
      CW(2,4,3)=0.1458262E-02                                           ABSOR  388
      CW(2,4,4)=0.3851421E-02                                           ABSOR  389
      CW(3,1,1)=0.5341917E-01                                           ABSOR  390
      CW(3,1,2)=-0.9407693E-01                                          ABSOR  391
      CW(3,1,3)=0.4356611E-02                                           ABSOR  392
      CW(3,1,4)=C.1492038E-02                                           ABSOR  393
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      CW(3,2,1)=-0.4708178E-02                                          ABSOR    394
      CW(3,2,2)=0.2086886E-01                                           ABSOR    395
      CW(3,2,3)=-0.9477933E-02                                          ABSOR    396
      CW(3,2,4)=0.6153272E-03                                           ABSOR    397
      CW(3,3,1)=-0.2104622E-01                                          ABSOR    398
      CW(3,3,2)=0.7515796E-02                                           ABSOR    399
      CW(3,3,3)=0.5965509E-02                                           ABSOR    400
      CW(3,3,4)=-0.2756144E-02                                          ABSOR    401
      CW(3,4,1)=0.4318975E-02                                           ABSOR    402
      CW(3,4,2)=-0.1005744E-01                                          ABSOR    403
      CW(3,4,3)=0.4091084E-03                                           ABSOR    404
      CW(3,4,4)=0.2990435E-02                                           ABSOR    405
    4 CONTINUE                                                          ABSOR    406
      X=ALOG(P)/3.45+1.0                                                ABSOR    407
      Y=(ALOG(PL)+2.555)/4.345                                          ABSOR    408
      Z=(T-1150.)/ 850.                                                 ABSOR    409
      V=0.0                                                             ABSOR    410
      DO 5 II=1,3                                                       ABSOR    411
      I=II-1                                                            ABSOR    412
      CALL CHEBY(I,X,TIX)                                               ABSOR    413
      V6=0.0                                                            ABSOR    414
      DO 6 JJ=1,4                                                       ABSOR    415
      J=JJ-1                                                            ABSOR    416
      CALL CHEBY(J,Y,TJY)                                               ABSOR    417
      V7=0.0                                                            ABSOR    418
      DO 7 KK=1,4                                                       ABSOR    419
      K=KK-1                                                            ABSOR    420
      CALL CHEBY(K,Z,TKZ)                                               ABSOR    421
      IF(INDEX.EQ.1)SC(II,JJ,KK)=CC(II,JJ,KK)                          ABSOR    422
      IF(INDEX.EQ.2)SC(II,JJ,KK)=CW(II,JJ,KK)                          ABSOR    423
      V7=V7+TKZ*SC(II,JJ,KK)                                            ABSOR    424
    7 CONTINUE                                                          ABSOR    425
      V6=V6+V7*TJY                                                      ABSOR    426
    6 CONTINUE                                                          ABSOR    427
      V=V+V6*TIX                                                        ABSOR    428
    5 CONTINUE                                                          ABSOR    429
      V=EXP(V)                                                          ABSOR    430
      RETURN                                                            ABSOR    431
      END                                                               ABSOR    432
      SUBROUTINE SOLVE                                                  SO         2
      COMMON/COEFF/AP(40),BP(40),EP(30),DP(30),APP(30),BPP(30)          NASAX     45
      COMMON F(3500),DU(500),DV(500),DW(500),                           COMFB      2
     1 ANUC(500),SOOT1(500),SOOT2(500),FCH(500),FH2(500),FS(500,14),    &STEP     18
     1 RHO(500),VISC(500),ABSR(500),SCTR(500),SU(100),SP(100),          RAD        3
     1 DRHODP(500),                                                     RAD        4
     1   AXP(100),AXM(100),AYP(100),AYM(100),AZP(100),                  COMFB      4
     2   AZM(100),CZ(100),CY(10),CZU(100),CYU(10),                      COMFB      5
     3   CZP(100),CYP(10),DIVG(100),NTP1,NTP2                           COMFB      6
     1,AXMK(192),AXPK(192),AYMK(192),AYPK(192),AZMK(192),AZPK(192),     CTDMA      3
     2 SUK(192),SPK(192)                                                CTDMA      4
      DIMENSION U(500),V(500),W(500),PP(500),P(500),TEMP(500)           COMFB      7
      DIMENSION GAM(500)                                                COMFB      8
      EQUIVALENCE (F(1),U(1)),(F(501),V(1)),(F(1001),W(1))              COMFB      9
      EQUIVALENCE (F(1501),PP(1)),(F(2001),P(1)),(F(2501),TEMP(1))      COMFB     10
      EQUIVALENCE (F(3001),GAM(1))                                      COMFB     11
      COMMON/CYL/R(30),RM(30),RMV(30),YSR(30),YSVR(30),IPLAX            COMMON     2
      COMMON/GRID/X(40),Y(30),Z(30),XS(40),YS(30),ZS(30),XSU(40),       COMMON     3
     1   YSV(30),ZSW(30),XDIF(40),YDIF(30),ZDIF(30),FXP(40),FXM(40),    COMMON     4
     2   FYP(30),FYM(30),FZP(30),FZM(30),DT,TIME                        COMMON     5
      COMMON                                                            NOX        2
     1/CINDEX/IDCC,IDFU,IDO2,IDN2,IDH2O,IDCO2,IDH1,IDH2,IDN1,IDNO,IDNO2 NOX        3
     1,IOO,IODH,IHCPS,ILC,ILH,IMAT,ITER,JJJ,N1,N2,N3,NA,NGLOB,NGLOBP,   NOX        4
     2 NLM,NO,NSP,NS1,NS2,IDCH                                          &STEP      3
     3/CCHEM1/CPSUM,HSUM,FQ,PPLN,RGAS,RGASIN,SMINV,TKINV,TLN,LNRG       NOX        6
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     4/CPARAM/ASUB(30,3),ENV,ER,HSUB0,NDEBUG,NS,PA,Q0,Q1,Q2,Q3,Q4,RHOPP,  NOX          7
     4 SM,SMW(30),SMO,S1(30),S2(30),TK,LADIAB,LDEBUG,LEQUIL,LREACT,      NOX          8
     4 LENER,EDKIJ,LCONVG                                                NOX          9
      DOUBLE PRECISION CPSUM,ENV,ER,FQ,HSUB0,HSUM,PA,PPLN,Q0,Q1,Q2,Q3,   NOX         10
     1 Q4,RGAS,RGASIN,RHOPP,SM,SMINV,SMW,S1,S2,TK,TKINV,TLN,SMO          NOX         11
     2,FUT,FST                                                           4STEP        4
      COMMON/STEP4/PEXP1,PEXP2,PEXP3,PEXP4,ER1,ER2,ER3,ER4,CEBU1,CEBU2,  4STEP        5
     1 CEBU3,CEBU4,AEXP1,AEXP2,AEXP3,AEXP4,BEXP1,BEXP2,BEXP3,BEXP4,      4STEP        6
     2 CEXP1,CEXP2,CEXP3,CEXP4,FUT,FST                                   4STEP        7
      LOGICAL LADIAB,LCONVG,LDEBUG,LEQUIL,LNRG,LREACT,LENER              NOX         12
      COMMON/INT/L,M,N,LCV,MCV,NCV,LP1,MP1,NP1,NI,NJ,NK,NINJ,NINJNK,NV,  COMMON      6
     1 NNV,NGOTO,K,ISTR,JSTR,KSTR,NVM(35),KM(30),JM(30),ISTEP,           4STEP        8
     2 ISOLVE(32),IPRINT(33),TITLE(10,33),IXY,ISWP,JSWP,RELAX(35),NP,    4STEP        9
     3  NRHO,NGAM,IWLI(30,5),IWLO(30,5),JWLO(40,5),JWLI(40,5),IWEI,      COMMON       9
     4  IWEO,MM1,JWII,JWIO,JWOI,JWOO,IDW,JKIN(30,30),IKIN(40,30)         COMMON      10
      COMMON/INDEX/IPAR,LPREF,ISTUN,INCOMP,ITRAD,NVRX,NVRY,NVRZ,JPLANE   COMMON      11
     1,PLAXM1,LVK,LVO,LVFUOX,LVFU,LVCO,LVH,LVRX,LVRY,LVRZ,NVF(32),       4STEP       10
     2  IJUMP,IRES,TITLE2(20),IMAX,JMAX,KMAX,NVCO,FUMCO,NVH2O,NVCO2,     COMMON      13
     3 NVN2,NVCH,NVH2                                                    4STEP       11
      COMMON/CNOX/LVH1,LVH2,LVN1,LVNO,LVNO2,LVO,LVOH,LVH2O,LVN2,LVO2,    NOX         16
     1 LVCO2,LVFU1,LVCO1,NNOX,INOX,ITNOX,SNOX,TNOX                       NOX         17
      COMMON/THERM/NVH,NVFU,NVOX,NVFUOX,NVTE,MODEN,IDK,FSTOIC,HFU,CP,    COMMON      15
     1  GASCON,RHOCON,UNICON,PRESS,NVFAV,TCYLW,TINLW,TLIP,ACOEF(4),      COMMON      16
     2  T4,DFAC,WFU,WCO2,WCO,WOX,WH2O,WN2,HYY,CXX,RATIO1,RATIO2,         COMMON      17
     3  RATIO3,RATIO4,HCO,TAN,ITWALL                                     COMMON      18
      COMMON/CTDMA/KEND,ICTDMA(32)                                       4STEP       12
C-----SUBROUTINE SOLVE IS USED TO SOLVE THE FINITE-DIFFERENCE            COMMENT    184
C     EQUATIONS BY THE TRI-DIAGONAL-MATRIX-ALGORITHM(TDMA).              COMMENT    185
C                                                                        COMMENT    186
      ENTRY SOLVE1                                                       SO           7
      RELAXM=1.-RELAX(NV)                                                SO           8
      DO 10 J=JSTR,M                                                     SO           9
      KJM=KM(K)+JM(J)                                                    SO          10
      IS=IWLI(J,NGOTO)                                                   SO          11
      IE=IWLO(J,NGOTO)                                                   SO          12
      DO 10 I=IS,IE                                                      SO          13
      LIJ=JM(J)+I                                                        SO          14
      LP=KJM+I                                                           SO          15
      LPF=LP+NVM(NVF(NV))                                                SO          16
      LZP=LPF+NINJ                                                       SO          17
      LZM=LPF-NINJ                                                       SO          18
      FLZP=F(LZP)                                                        SO          19
      IF (NV.EQ.3.AND.K.EQ.NP1) FLZP=W(LIJ+2*NINJ)                       SO          20
10    CONTINUE                                                           SO          21
      SP(LIJ)=(AXM(LIJ)+AXP(LIJ)+AYM(LIJ)+AYP(LIJ)+AZM(LIJ)+AZP(LIJ)-    SO          22
     1SP(LIJ))/RELAX(NV)                                                 SO          23
C-----STORE COEFFICIENTS FOR CYCLIC TDMA.                                COMMENT    187
      LPC=I-1+(J-2)*(NI-2)+(K-KSTR)*(NI-2)*(NJ-2)                        CTDMA        5
      AYMK(LPC)=AXP(LIJ)                                                 CTDMA        6
      AXPK(LPC)=AXP(LIJ)                                                 CTDMA        7
      AYMK(LPC)=AYM(LIJ)                                                 CTDMA        8
      AYPK(LPC)=AYP(LIJ)                                                 CTDMA        9
      AZMK(LPC)=AZM(LIJ)                                                 CTDMA       10
      AZPK(LPC)=AZP(LIJ)                                                 CTDMA       11
      SUK(LPC)=SU(LIJ)+SP(LIJ)*RELAXM*F(LPF)                             CTDMA       12
      SPK(LPC)=SP(LIJ)+1.0E-30                                           CTDMA       13
      SU(LIJ)=SU(LIJ)+SP(LIJ)*RELAXM*F(LPF)+AZM(LIJ)*F(LZM)+AZP(LIJ)*    SO          24
     1  FLZP                                                             SO          25
      GO TO (11,12,13,10),NGOTO                                          SO          26
   11 DU(LP)=DU(LP)/SP(LIJ)                                              SO          27
      GO TO 10                                                           SO          28
   12 DV(LP)=DV(LP)/SP(LIJ)                                              SO          29
      GO TO 10                                                           SO          30
   13 DW(LP)=DW(LP)/SP(LIJ)                                              SO          31
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10    CONTINUE                                                                  SO        32
      NVKM=KM(K)+NVP(NVF(NV))                                                   SO        33
      ISUM=ISTP+L                                                               SO        34
      JSUM=JSTR+M                                                               SO        35
      INOMAX=ICTOMA(NV)                                                         SO        36
      DO 45 INO=1,INOMAX                                                        SO        37
      GO TO (20,30),IXY                                                         SO        38
20    CONTINUE                                                                  SO        39
C-----TOMA TRAVERSE IN X-DIRECTION.                                             COMMENT   188
      DO 21 JJ=JSTR,M                                                           SO        40
      GO TO (24,25),JSWP                                                        SO        41
24    J=JJ                                                                      SO        42
      GO TO 26                                                                  SO        43
25    J=JSUM-JJ                                                                 SO        44
26    CONTINUE                                                                  SO        45
      LPF=NVKM+JM(J)                                                            SO        46
      IS=IWLI(J,NGOTO)                                                          SO        47
      IE=IWLO(J,NGOTO)                                                          SO        48
      ISTR1=IS-1                                                                SO        49
      LPF1=LPF+ISTR1                                                            SO        50
      AP(ISTR1)=0.                                                              SO        51
      BP(ISTR1)=F(LPF1)                                                         SO        52
      DO 22 I=IS,IE                                                             SO        53
      LIJ=JM(J)+I                                                               SO        54
      LYP=LPF+NI+I                                                              SO        55
      LYM=LPF-NI+I                                                              SO        56
      STORE=SP(LIJ)-AXM(LIJ)*AP(I-1)+1.E-30                                     SO        57
      AP(I)=AXP(LIJ)/STORE                                                      SO        58
22    BP(I)=(SU(LIJ)+AYP(LIJ)*F(LYP)+AYM(LIJ)*F(LYM)+AXM(LIJ)*BP(I-1))/        SO        59
     1STORE                                                                     SO        60
      ISUM1=IS+IE                                                               SO        61
      DO 23 II=IS,IE                                                            SO        62
      I=ISUM1-II                                                                SO        63
      LP=LPF+I                                                                  SO        64
23    F(LP)=AP(I)*F(LP+1)+BP(I)                                                 SO        65
21    CONTINUE                                                                  SO        66
      JSWP=3-JSWP                                                               SO        67
      GO TO (28,20),JSWP                                                        SO        68
   28 CONTINUE                                                                  SO        69
      GO TO (30,40),IXY                                                         SO        70
C-----TOMA TRAVERSE IN Y-DIRECTION.                                             COMMENT   189
30    DO 31 II=ISTR,L                                                           SO        71
      GO TO (34,35),ISWP                                                        SO        72
34    I=II                                                                      SO        73
      GO TO 36                                                                  SO        74
35    I=ISUM-II                                                                 SO        75
36    CONTINUE                                                                  SO        76
      LPF=NVKM+I                                                                SO        77
      JS=JWLI(I,NGOTO)+1                                                        SO        78
      JE=JWLO(I,NGOTO)-1                                                        SO        79
      JSTR1=JS-1                                                                SO        80
      LPF1=LPF+JM(JSTR1)                                                        SO        81
      AP(JSTR1)=0.                                                              SO        82
      BP(JSTR1)=F(LPF1)                                                         SO        83
      DO 32 J=JS,JE                                                             SO        84
      LIJ=JM(J)+I                                                               SO        85
      LXP=NVKM+LIJ+1                                                            SO        86
      LXM=LXP-2                                                                 SO        87
      STORE=SP(LIJ)-AYM(LIJ)*AP(J-1)+1.E-30                                     SO        88
      AP(J)=AYP(LIJ)/STORE                                                      SO        89
32    BP(J)=(SU(LIJ)+AXP(LIJ)*F(LXP)+AXM(LIJ)*F(LXM)+AYM(LIJ)*BP(J-1))/        SO        90
     1STORE                                                                     SO        91
      JSUM1=JS+JE                                                               SO        92
      DO 33 JJ=JS,JE                                                            SO        93
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      J=JSUM1-JJ                                                        SO         94
      LP=LPF+JM(J)                                                      SO         95
      LYP=LP+NI                                                         SO         96
   33 F(LP)=AP(J)*F(LYP)+BP(J)                                          SO         97
   31 CONTINUE                                                          SO         98
      ISWP=3-ISWP                                                       SO         99
      GO TO (30,30),ISWP                                                SO        100
   30 CONTINUE                                                          SO        101
      GO TO (40,20),IXY                                                 SO        102
   40 CONTINUE                                                          SO        103
   45 CONTINUE                                                          SO        104
      RETURN                                                            SO        105
C  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  **  * SO        106
      ENTRY SOLVE2                                                      SO        107
C-----CYCLIC TDMA IN Z-DIRECTION.                                       COMMENT   190
      KEND=N                                                            CTDMA      14
      IF(NV.EQ.3)KEND=NP1                                               CTDMA      15
      IF(ICTDMA(NV).EQ.0)GO TO 606                                      CTDMA      16
      INDMAX=ICTDMA(NV)                                                 CTDMA      17
      DO 605 IND=1,INDMAX                                               CTDMA      18
      DO 600 J=JSTR,M                                                   CTDMA      19
      IS=IWLI(J,NGOTO)                                                  FEB2        4
      IE=IWLO(J,NGOTO)                                                  FEB2        5
      DO 600 I=IS,IE                                                    FEB2        6
      LIJ=I+JM(J)                                                       CTDMA      21
      LIJNV=LIJ+NVM(NVF(NV))                                            CTDMA      22
      LPSTR=LIJNV+KM(KSTR)                                              CTDMA      23
      LPCSTR=I-1+(J-2)*(NI-2)                                           CTDMA      24
      AP(KSTR)=AZPK(LPCSTR)                                             CTDMA      25
      BP(KSTR)=AZMK(LPCSTR)                                             CTDMA      26
      FP(KSTR)=SUK(LPCSTR)+AXMK(LPCSTR)*F(LPSTR-1)+AXPK(LPCSTR)*F(LPSTR+ CTDMA      27
     21)+AYMK(LPCSTR)*F(LPSTR-NI)+AYPK(LPCSTR)*F(LPSTR+NI)              CTDMA      28
      DP(KSTR)=SPK(LPCSTR)                                              CTDMA      29
      IF(DP(KSTR).LT.1.E-30)DP(KSTR)=1.E30                              CTDMA      30
      KMIN=KSTR+1                                                       CTDMA      31
      DO 601 K=KMIN,KEND                                                CTDMA      32
      LPC=I-1+(J-2)*(NI-2)+(K-KSTR)*(NI-2)*(NJ-2)                       CTDMA      33
      LP=LIJNV+KM(K)                                                    CTDMA      34
      AP(K)=AZPK(LPC)                                                   CTDMA      35
      BK=AZMK(LPC)                                                      CTDMA      36
      CK=SUK(LPC)+AXMK(LPC)*F(LP-1)+AXPK(LPC)*F(LP+1)+AYMK(LPC)*F(LP-NI) CTDMA      37
     2    +AYPK(LPC)*F(LP+NI)                                           CTDMA      38
      DK=SPK(LPC)                                                       CTDMA      39
      BP(K)=BK*BP(K-1)/DP(K-1)                                          CTDMA      40
      FP(K)=FP(K-1)*BK/DP(K-1)+CK                                       CTDMA      41
      DP(K)=DK-BK*AP(K-1)/DP(K-1)                                       CTDMA      42
      IF(DP(K).LT.1.E-30)DP(K)=1.E30                                    CTDMA      43
  601 CONTINUE                                                          CTDMA      44
      KSUM=KEND-2+KSTR                                                  CTDMA      45
      APP(KEND-1)=(AP(KEND-1)+BP(KEND-1))/DP(KEND-1)                    CTDMA      46
      BPP(KEND-1)=FP(KEND-1)/DP(KEND-1)                                 CTDMA      47
      KENDM2=KEND-2                                                     CTDMA      48
      DO 602 KK=KSTR,KENDM2                                             CTDMA      49
      K=KSUM-KK                                                         CTDMA      50
      APP(K)=(AP(K)*APP(K+1)+BP(K))/(DP(K)+1.0E-30)                     CTDMA      51
      BPP(K)=(AP(K)*BPP(K+1)+FP(K))/(DP(K)+1.0E-30)                     CTDMA      52
  602 CONTINUE                                                          CTDMA      53
      DENOM=DP(KEND)-BP(KEND)-APP(KSTR)*AP(KEND)                        CTDMA      54
      IF(ABS(DENOM).LT.1.E-30)DENOM=1.E30                               CTDMA      55
      FEND=(BPP(KSTR)*AP(KEND)+FP(KEND))/DENOM                          CTDMA      56
      KENDM1=KEND-1                                                     CTDMA      57
      DO 603 K=KSTR,KENDM1                                              CTDMA      58
      LP=LIJNV+KM(K)                                                    CTDMA      59
      F(LP)=APP(K)*FEND+BPP(K)                                          CTDMA      60
244
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  603 CONTINUE                                                          CTDMA      61
      LPCE=LIJNV+KM(KEND)                                               CTDMA      62
      F(LPCE)=FEND                                                      CTDMA      63
  600 CONTINUE                                                          CTDMA      64
  602 CONTINUE                                                          CTDMA      65
  606 CONTINUE                                                          CTDMA      66
      RETURN                                                            SD        108
      END                                                               SD        109
      SUBROUTINE FPRINT (ISTRT,ISTOP,NVVV)                              FP          2
      COMMON F(3500),DU(500),DV(500),DW(500),                           COMFB       2
     1 ANUC(500),SQOT1(500),SQOT2(500),FCN(500),FH2(500),FS(500,14),    4STEP      10
     1 RHO(500),VISC(500),ABSR(500),SCTR(500),SU(100),SP(100),          RAD         3
     1 DRHODP(500),                                                     RAD         4
     1  AXP(100),AXM(100),AYP(100),AYM(100),AZP(100),                   COMFB       4
     2  AZM(100),CZ(100),CY(10),CZU(100),CYU(10),                       COMFB       5
     3  CZP(100),CYP(10),DIVG(100),NTP1,NTP2                            COMFB       6
     1,AXMK(192),AXPK(192),AYMK(192),AYPK(192),AZMK(192),AZPK(192),     CTDMA       3
     2 SUK(192),SPK(192)                                                CTDMA       4
      DIMENSION U(500),V(500),W(500),PP(500),P(500),TEMP(500)           COMFB       7
      DIMENSION GAM(500)                                                COMFB       8
      EQUIVALENCE (F(1),U(1)),(F(501),V(1)),(F(1001),W(1))              COMFB       9
      EQUIVALENCE (F(1501),PP(1)),(F(2001),P(1)),(F(2501),TEMP(1))      COMFB      10
      EQUIVALENCE (F(3001),GAM(1))                                      COMFB      11
      COMMON/CYL/R(30),RM(30),RMV(30),YSR(30),YSVR(30),IPLAX            COMMON      2
      COMMON/GRID/X(40),Y(30),Z(30),XS(40),YS(30),ZS(30),XSU(40),       COMMON      3
     1  YSV(30),ZSW(30),XDIF(40),YDIF(30),ZDIF(30),FXP(40),FXM(40),     COMMON      4
     2  FYP(30),FYM(30),FZP(30),FZM(30),DT,TIME                         COMMON      5
      COMMON                                                            NOX         2
     1/CTNOFX/IDCO,IDFU,IDO2,IDN2,IDH2O,IDCO2,IDH1,IDH2,IDN1,IDNO,IDNO2 NOX         3
     1,IDO,IDOH,IHCPS,ILC,ILH,IMAT,ITER,JJJ,N1,N2,N3,NA,NGLOB,NGLOBP,   NOX         4
     2 NLM,NQ,NSM,NS1,NS2,IDCH                                          4STEP       3
     3/CCHEMI/CPSUM,HSUM,FQ,PPLN,RGAS,RGASIN,SMINV,TKINV,TLN,LNRG       NOX         6
     4/CPARAM/ASUB(30,3),ENV,ER,HSUBO,NDEBUG,NS,PA,QQ,Q1,Q2,Q3,Q4,RHOPP, NOX         7
     4 SM,SMN(30),SMO,S1(30),S2(30),TK,LADIAB,LDEBUG,LEQUIL,LREACT,     NOX         8
     4 LENER,EDKID,LCONVG                                               NOX         9
      DOUBLE PRECISION CPSUM,ENV,ER,FQ,HSUBO,HSUM,PA,PPLN,QQ,Q1,Q2,Q3,  NOX        10
     1 Q4,RGAS,RGASIN,RHOPP,SM,SMINV,SMW,S1,S2,TK,TKINV,TLN,SMO         NOX        11
     2,FUT,FST                                                          4STEP       4
      COMMON/STEP4/PEXP1,PEXP2,PEXP3,PEXP4,ER1,ER2,ER3,ER4,CEBU1,CEBU2, 4STEP       5
     1 CEBU3,CEBU4,AEXP1,AEXP2,AEXP3,AEXP4,BEXP1,BEXP2,BEXP3,BEXP4,     4STEP       6
     2 CEXP1,CEXP2,CEXP3,CEXP4,FUT,FST                                  4STEP       7
      LOGICAL LADIAB,LCONVG,LDEBUG,LEQUIL,LNRG,LREACT,LENER             NOX        12
      COMMON/INT/L,M,N,LCV,MCV,NCV,LP1,MP1,NP1,NI,NJ,NK,NINJ,NINJNK,NV,  COMMON      6
     1 NNV,NGOTO,K,ISTR,JSTR,KSTR,NVM(35),KM(30),JM(30),ISTEP,          4STEP       8
     2 ISOLVE(32),IPRINT(33),TITLE(10,33),IXY,ISWP,JSWP,RELAX(35),NP,   4STEP       9
     3  NRHO,NGAM,IWLI(30,5),IWLO(30,5),JWLO(40,5),JWLI(40,5),IWEI,     COMMON      9
     4  IWEO,PM1,JWII,JWIO,JWOI,JWOO,IDW,JKIN(30,30),IKIN(40,30)        COMMON     10
      COMMON/INDEX/IPAP,LPREF,ISTUN,INCONP,ITRAD,NVRX,NVRY,NVRZ,JPLANE  COMMON     11
     1,PLAXM1,LVK,LVD,LVFUOX,LVFU,LVCO,LVH,LVRX,LVRY,LVRZ,NVF(32),      4STEP      10
     2  IJUMP,IRES,TITLE2(20),IMAX,JMAX,KMAX,NVCO,FUNCO,NVH2O,NVCO2,    COMMON     13
     3 NVN2,NVCH,NVH2                                                   4STEP      11
      COMMON/CNOX/LVH1,LVH2,LVN1,LVNO,LVNO2,LVO,LVOH,LVH2O,LVN2,LVO2,   NOX        16
     1 LVCO2,LVFU1,LVCO1,NNOX,INOX,ITNOX,SNOX,TNOX                      NOX        17
      COMMON/THERM/NVH,NVFU,NVOX,NVFUOX,NVTE,NODEN,IDK,FSTOIC,HFU,CP,   COMMON     15
     1  GASCON,RHOCON,UNICON,PRESS,NVFAV,TCYLW,TINLW,TLIP,ACOEF(4),     COMMON     16
     2  T4,OFAC,WFU,WCO2,WCO,WOX,WH2O,WN2,HYY,CXX,RATIO1,RATIO2,        COMMON     17
     3  RATIO3,RATIO4,HCO,TAM,ITWALL                                    COMMON     18
      COMMON/CTDMA/KEND,ICTDMA(92)                                      4STEP      12
C-----SUBROUTINE FPRINT IS USED TO PRINT THE FIELD VALUES OF            COMMENT   191
C     ALL THE DEPENDENT VARIABLES.                                      COMMENT   192
C                                                                       COMMENT   193
      NVV=NVVV-1                                                        FP          7
      DO 108 NV=ISTRT,ISTOP                                             FP          8
      NVV=NVV+1                                                         FP          9
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      IF (IPRINT(NVV).EQ.0) GO TO 108                                    FP        10
      WRITE (6,101) (TITLE(I,NVV),I=1,10)                                FP        11
  101 FORMAT (1HC,20(2H0-),10A4,3X,20(2H-0))                             FP        12
      KONE=1                                                             FP        13
      IF (NVV.EQ.3) KONE=2                                               FP        14
      NSKIP=IPRINT(NVV)                                                  FP        15
      DO 100 K=KONE,NP1,NSKIP                                            FP        16
      WRITE(6,102) K                                                     FP        17
  102 FORMAT(1HO,58X,4HK = ,I2)                                          FP        18
      NVKM=NVM(NV)+KM(K)                                                 FP        19
      JONE=1                                                             FP        20
      IF (NVV.EQ.2) JONE=2                                               FP        21
      IONE=1                                                             FP        22
      IF (NVV.EQ.1) IONE=2                                               FP        23
      ISTART=IONE-12                                                     FP        24
  105 CONTINUE                                                           FP        25
      ISTART=ISTART+12                                                   FP        26
      IEND=ISTART+11                                                     FP        27
      IEND=MIND(IEND,LP1)                                                FP        28
      WRITE(6,103) (I,I=ISTART,IEND)                                     FP        29
  103 FORMAT(1HO,6H   I = ,I3,11I10)                                     FP        30
      WRITE(6,104)                                                       FP        31
  104 FORMAT(2H J)                                                       FP        32
      JSUM=JONE+NP1                                                      FP        33
      DO 106 JJ=JONE,NP1                                                 FP        34
      J=JSUM-JJ                                                          FP        35
      LPF=NVKM+JM(J)                                                     FP        36
      LPL=LPF+IEND                                                       FP        37
      LPF=LPF+ISTART                                                     FP        38
  106 WRITE(6,107) J,(F(LP),LP=LPF,LPL)                                  FP        39
  107 FORMAT(I3,1P12E10.2)                                               FP        40
      IF(IEND.LT.LP1) GO TO 105                                          FP        41
  100 CONTINUE                                                           FP        42
  108 CONTINUE                                                           FP        43
       RETURN                                                            FP        44
          END                                                            FP        45
      SUBROUTINE CREK                                                    NOXXX      1
C                                                                        CREK       3
C                                                                        CREK       4
C  A COMPUTER PROGRAM FOR CALCULATION OF                                 CREK       5
C  CHEMICAL REACTION EQUILIBRIUM AND KINETICS                            CREK       6
C  IN LAMINAR OR TURBULENT FLOWS                                         CREK       7
C                                                                        CREK       8
C  CALLING PROGRAM MUST FIRST EXPRESS SPECIES AND ENERGY CONSERVATION    CREK       9
C  FINITE-DIFFERENCE EQUATIONS IN THE STANDARD FORMS                     CREK      10
C                                                                        CREK      11
C     AP*S2(I),P = AE*S2(I),E + AW*S2(I),W + AN*S2(I),N + AS*S2(I),S     CREK      12
C                  +AH*S2(I),H + AL*S2(I),L + SO(S2(I)) ,   I=1,NS       CREK      13
C  DEPT M.E.   WASHINGTON STATE UNIVERSITY                               CREK      14
C  PULLMAN, WASHINGTON 99163                                             CREK      15
C  MARCH 1976                                                            CREK      16
C  DAVID T. PRATT AND JOHN J. MORNECK                                    CREK      17
C                                                                        CREK      18
C                                                                        CREK      19
C  ***SUMMARY***                                                         CREK      20
C  CREK CONSISTS OF 5 FORTRAN-IV SUBROUTINES& CREK,CREKO,SPECE,CALC,HCPS CREK      21
C  WHICH ENABLES THE EXTENSION OF ANY EXISTING HYDRODYNAMIC COMPUTER     CREK      22
C  CODE TO THE CALCULATION OF COMPLEX FLOW WITH CHEMICALLY COMPLEX       CREK      23
C  EQUILIBRIUM OR KINETIC STATIONARY STATES                              CREK      24
C  THIS VERSION OF CREK IS LIMITED TO IDEAL HOMOGENEOUS GAS-PHASE        CREK      25
C  CHEMICAL EQUILIBRIUM AND NON-EQUILIBRIUM (KINETIC) STATES             CREK      26
C                                                                        CREK      27
C  ***CALLING CREK*M*                                                    CREK      28
C  CALLING PROGRAM SEEKS SOLUTION FOR VALUES AT A POINT P OF MOLE        CREK      29
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C  NUMBERS OF CHEMICAL SPECIES, (S2(I),I=1,NS) AND THE TEMPERATURE TK,      CREK   30
C  GIVEN THE VALUES OF SAME VARIABLES AT NEIGHBORING NODES, AND VALUES      CREK   31
C  AT P AT A PREVIOUS TIME STEP OR ESTIMATES FROM PREVIOUS ITERATION        CREK   32
C                                                                           CREK   33
C  WHERE                                                                    CREK   34
C        AP = AE + AW + AN + AS + AH + AL + APP                             CREK   35
C        AO DENOTES CONVECTIVE AND DIFFUSIVE FLUX COEFFICIENTS              CREK   36
C             AT NEIGHBORING NODES O=E,W,N,S,H AND L, KG/CU M-SEC           CREK   37
C        APP IS INFLUENCE TERM FROM P AT PREVIOUS TIME STEP                 CREK   38
C        S2(I) IS THE MOLE NO. OF SPECIES I AT THE POINT P, KG-MOLEI/KG     CREK   39
C        S2(I),O IS THE MOLE NO. OF SPECIES I AT NEAR-NODE O,               CREK   40
C             KG-MOLE I/KG                                                  CREK   41
C        SO(S2(I)) IS RATE OF APPEARANCE OF SPECIES I DUE TO                CREK   42
C             CHEMICAL REACTION, KG-MOLES I/CU M-SEC                        CREK   43
C                                                                           CREK   44
C  AND                                                                      CREK   45
C                                                                           CREK   46
C     AP*H,P = AE*H,E + AW*H,W + AN*H,N + AS*H,S + AH*H,H + AL*H,L          CREK   47
C              + SO(H)                                                      CREK   48
C  WHERE                                                                    CREK   49
C        H,P IS THE MIXTURE ENTHALPY AT POINT P, J/KG                       CREK   50
C        H,O IS THE MIXTURE ENTHALPY AT NEIGHBOR NODES O,                   CREK   51
C        SO(H) IS RATE OF HEAT ADDITION TO CONTROL VOLUME BY                CREK   52
C             RADIATIVE AND KINETIC HEATING, J/CU M-SEC                     CREK   53
C                                                                           CREK   54
C  CALLING PROGRAM MUST SUPPLY FOLLOWING VARIABLES THROUGH LABELLED         CREK   55
C  COMMON BLOCK /CPARAM/                                                    CREK   56
C                                                                           CREK   57
C        TK = TEMPERATURE AT NODE P, DEGREES KELVIN (ESTIMATE)              CREK   58
C        PA = PRESSURE AT POINT P, PASCALS (NT/SQ M)                        CREK   59
C        FMV = AP, KG/CU M-SEC                                              CREK   60
C        S1(I) = (AE*S2(I),E+AW*S2(I),W...+AL*S2(I),L) / AP                 CREK   61
C  *     S2(I) = PREVIOUS SOLUTIONS OR ESTIMATES FOR S2(I)...    *          CREK   62
C ***            IF TEMP TK IS SET TO ZERO, PROGRAM CONSTRUCTS  ***         CREK   63
C ***            OWN ESTIMATES                                  ***         CREK   64
C  *     HSUBO = (AE*H,E+AW*H,W...+AL*H,L) / AP     , J/KG       *          CREK   65
C        00,01,02,03,04, = COEFFICIENTS IN EXPRESSION FOLLOWING...          CREK   66
C        SO(H) = -(00+01*T+02*T**2+03*T**3+04*T**4) , J/CU M-SEC            CREK   67
C                                                                           CREK   68
C  LADIAB = T ---  IGNORES ABOVE EXPRESSION FOR SO(H), TAKES                CREK   69
C                  SOURCE(H)=0.0                                            CREK   70
C  LEQUIL = T ---  EQUILIBRIUM SOLUTION SOUGHT                              CREK   71
C         = F ---  KINETIC SOLUTION SOUGHT                                  CREK   72
C  LREACT = T ---  CHEMICAL REACTION (EQL OR KIN)                           CREK   73
C         = F ---  ADIABATIC NON-REACTING MIXING                            CREK   74
C  LDEBUG = T ---  INTERMEDIATE DEBUG PRINTING                              CREK   75
C         = F ---  NO INTERMEDIATE DEBUG PRINTING                           CREK   76
C                                                                           CREK   77
C  ***RETURN***                                                             CREK   78
C  S2(I),I=1,NS  IS THE MOLE NUMBER OF CHEMICAL SPECIES I (KG-MOLE I/KG)    CREK   79
C  TK IS THE TEMPERATURE (DEGREES K) FROM THERMAL ENERGY EQUATION           CREK   80
C  HSUBO IS STATIC ENTHALPY AT NODE POINT P  (J/KG)                         CREK   81
C  RHOP IS THE MASS DENSITY AT NODE POINT P  (KG/CU M)                      CREK   82
C  SM IS RECIPROCAL OF MIXTURE MOLECULAR WEIGHT  (KG-MOLE/KG)               CREK   83
C  ASUB(I,3) IS THE SPECIES NAME (HOLLERITH FIELD)                          CREK   84
C                                                                           CREK   85
C  ***DIMENSIONS***                                                         CREK   86
C        NLM = NUMBER OF ELEMENTS (7)                                       CREK   87
C        NS  = NUMBER OF CHEMICAL SPECIES (20)                              CREK   88
C        JJ  = NUMBER OF CHEMICAL REACTIONS (36)                            CREK   89
C                                                                           CREK   90
C  THESE DIMENSIONS MAY BE ADJUSTED BY SIMPLY CHANGING THE                  CREK   91
C  FOLLOWING LABELLED COMMON BLOCKS&                                        CREK   92
C                                                                           CREK   93
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C         CEQUIL...NLM,NS                                                    CREK      94
C         CINDEX...                                                          CREK      95
C         CKINET...                                                          CREK      96
C         CMATRI...NS+2                                                      CREK      97
C         CPARAM...NS                                                        CREK      98
C         CREACT...JJ                                                        CREK      99
C         CSPECF...NS                                                        CREK     100
C                                                                            CREK     101
C   AND THE FOLLOWING DIMENSION STATEMENT IN ROUTINE CALC WHICH              CREK     102
C   SHOULD BE DOUBLE DIMENSIONED FOR IBM MACHINES                            CREK     103
C                                                                            CREK     104
C         A(NS+2,NS+3)                                                       CREK     105
C                                                                            CREK     106
C                                                                            CREK     107
C                                                                            CREK     108
      DOUBLE PRECISION AL,BO,CPSUM,ENV,ER,FQ,HSUBO,HSUM,HO,PA,PI,PPLN,       NOXX       1
     1 QO,Q1,Q2,Q3,Q4,RGAS,RGASIN,RHOP,SM,SMINV,SMW,SSAVE,SO,S1,S2,TK,        NOXXX      3
     2 TKINV,TLN,Z,SMO                                                       NOXXX      4
      DOUBLE PRECISION ENVSAV,FACTOR,SMALL,TSAVE,XHI,XLO                     NOXX       2
      LOGICAL LADIAB,LCONVG,LDEBUG,LEQUIL,LNRG,LREACT,LENER                  NOXX       3
C                                                                            CREK     113
      COMMON                                                                 CREK     114
     3/CCHEM1/CPSUM,HSUM,FQ,PPLN,RGAS,RGASIN,SMINV,TKINV,TLN,LNRG            NOXX       4
     1/CEQUIL/AL(7,30),ATOM(3,7),BO(7),PI(7)                                 CREK     116
     1/CINDEX/IDCO,IDFU,IDO2,IDN2,IDH2O,IDCO2,IDH1,IDH2,IDN1,IDNO,IDNO2      NOXX       5
     1,IDO,IDOH,IHCPS,ILC,ILH,IMAT,ITER,JJ,N1,N2,N3,NA,NGLOB,NGLOBP,         NOXX       6
     2 NLM,NO,NSM,NS1,NS2,IDCH                                               ASTER    344
     1/CPARAM/ASUB(30,3),ENV,ER,HSUBO,NDEBUG,NS,PA,QO,Q1,Q2,Q3,Q4,RHOP,      CREK     119
     1 SM,SMW(30),SMO,S1(30),S2(30),TK,LADIAB,LDEBUG,LEQUIL,LREACT,LEMER     NOXX       8
     2,FORIJ,LCONVG                                                          NOXX       9
     1/CSPECF/HO(30),SO(30),SSAVE(30),Z(7,2,30)                              NOXX      10
C                                                                            CREK     122
C*************************************************************************** CREK     123
C  THIS SUBROUTINE IS THE MAIN EQUILIBRIUM AND KINETIC SOLUTION ROUTINE.     CREK     124
C  THE CALLING PROGRAM MUST SUPPLY ALL THE VARIABLES EXCEPT RHOP AND SM      CREK     125
C  THROUGH THE LABELLED COMMON BLOCK CPARAM IN SI UNITS.  BOTH EQUIL         CREK     126
C  SOLUTIONS (LEQUIL=.) -- BY MINIMIZATION OF THE GIBBS FUNCTION --          CREK     127
C  AND KINETIC (LEQUIL=F) SOLUTIONS ARE CALCULATED BY A NE.  .-RAPHSON       CREK     128
C  TECHNIQUE.  CREK ALSO CONTROLS THE LOGIC FOR PROBLEM CELLS                CREK     129
C  REFERENCE  CREK    (WASHINGTON STATE UNIVERSITY)  MARCH 1976              CREK     130
C*************************************************************************** CREK     131
C                                                                            CREK     132
      DATA FACTOR/5.000/,SMALL/1.00-6/                                       CREK     133
C                                                                            CREK     134
C                                                                            CREK     135
C  ***NORMAL SOLUTION***                                                     CREK     136
C                                                                            CREK     137
C  DETERMINE EQUIVALENCE RATIO AND IF OUTSIDE INTERVAL (0.1,10) ASSUME       CREK     138
C  NO REACTION AND RETURN ADIABATIC NON-REACTED MIXTURE PROPERTIES           CREK     139
C  SAVE GIVEN ESTIMATES OR PROGRAM GENERATED ESTIMATES IF TK IS SMALL        CREK     140
C  IF SOLUTION IS SUCCESSFUL, RETURN TO CALLING ROUTINE  OTHERWISE,          CREK     141
C  ENTER PROBLEM CELL LOGIC BELOW                                            CREK     142
      LCONVG=.TRUE.                                                          NOXX      11
C                                                                            CREK     143
      CALL EQATIC                                                            CREK     144
      IF (.NOT.LDEBUG) GO TO 30                                              CREK     145
      WRITE(6,10) LREACT,LEQUIL,LADIAB,ENV,ER,HSUBO,QO,Q1,Q2,Q3,Q4,PA,TK     CREK     146
   10 FORMAT(1X,3L3,1P10D12.3)                                               CREK     147
      IF (NDEBUG.EQ.1) GO TO 30                                              CREK     148
      WRITE(6,20) (S1(I),I=1,NS)                                             CREK     149
      WRITE(6,20) (S2(I),I=1,NS)                                             CREK     150
   20 FORMAT(1X,1P10D12.3)                                                   CREK     151
   30 IF (.NOT.LREACT) GO TO 400                                             CREK     152
      ENVSAV=ENV                                                             CREK     153
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C       11.526C9 IS E-LOG OF STD PATM=101325.0 N/M**2                    CREK     155
        PPLM=DLOG(PA)-11.5260 D0                                         CREK     156
        TSAVE=TK                                                         CREK     157
        DO 40 I=1,NS                                                     CREK     158
   40   SSAVE(I)=S2(I)                                                   CREK     159
        IF (TK.LT.SMALL) GO TO 100                                       CREK     160
C                                                                        CREK     161
        CALL SPECE                                                       CREK     162
C                                                                        CREK     163
        IF (LCONVG) GO TO 900                                            CREK     164
        DO 101 I=1,NS                                                    NOXX      12
        IF(S2(I).LT.2.00-20)S2(I)=S1(I)                                  NOXX      13
  101   CONTINUE                                                         NOXX      14
        IF(.NOT.LCONVG)GO TO 900                                         NOXX      15
C                                                                        CREK     165
C                                                                        CREK     166
C  ***PROBLEM CELL***                                                    CREK     167
C                                                                        CREK     168
C  SOLUTION LOGIC IS DIFFERENT FOR FOUR TYPES OF PROBLEMS AS FOLLOWS6    CREK     169
C     MODE 1 ... LEQUIL = T, LADIAB = T                                  CREK     170
C     MODE 2 ... LEQUIL = T, LADIAB = F                                  CREK     171
C     MODE 3 ... LEQUIL = F, LADIAB = T                                  CREK     172
C     MODE 4 ... LEQUIL = F, LADIAB = F                                  CREK     173
C                                                                        CREK     174
C  ALWAYS TRY RT=0.0 (LNRG=F) AFTER SOLUTION FAILURE WHEN LEQUIL=F.      CREK     175
C  LOGIC TO FIND SOLUTION IS CONTROLLED IN CHAPTERS 1 AND 2 BELOW        CREK     176
C  WHERE IN EACH SECTION, NEW ESTIMATES ARE DETERMINED EITHER BY         CREK     177
C  SAVED GIVEN ONES, NEW ASSIGNED ONES, OR SOLUTION FOUND NOT AT         CREK     178
C  REQUIRED CONDITIONS.  THE VARIABLES NEXTOK AND NEXTNG ARE ASSIGNED    CREK     179
C  THE STATEMENT NUMBERS OF WHERE TO GO IF THE SOLUTION ATTEMPT IS       CREK     180
C  SUCCESSFUL OR NOT, RESPECTIVELY.                                      CREK     181
C                                                                        CREK     182
        ASSIGN 900 TO NEXTOK                                             CREK     183
        ASSIGN 100 TO NEXTNG                                             CREK     184
        GO TO 520                                                        CREK     185
C                                                                        CREK     186
C* * * * * * * * * * * * * * * * * * * * * CHAPTER 1 * * * * * * *      CREK     187
C* * * * * * * * * * * * * * * * * * * * * CHAPTER 1 * * * * * * *      CREK     188
C                                                                        CREK     189
C  ***EQUILIBRIUM***                                                    CREK     190
C  THIS CHAPTER MAKES EQUILIBRIUM ESTIMATES AND INITIATES STRATEGY FOR   CREK     191
C  CASES IN WHICH CONVERGENCE WAS NOT ACHIEVED ON FIRST CALL TO SPECE    CREK     192
C                                                                        CREK     193
  100   MODE=4                                                           CREK     194
        IF (LEQUIL) MODE=MODE-2                                          CREK     195
        IF (LADIAB) MODE=MODE-1                                          CREK     196
        LEQUIL=.TRUE.                                                    CREK     197
        LADIAB=.TRUE.                                                    CREK     198
        IF (MODE.LT.3.OR.TK.LT.SMALL) GO TO 170                          CREK     199
C                                                                        CREK     200
C-----FIRST USE GIVEN ESTIMATES FOR EQUIL SOLN IN MODE 3 AND 4 PROBLEMS  CREK     201
C                                                                        CREK     202
        TK=TSAVE                                                         CREK     203
        DO 120 I=1,NS                                                    CREK     204
  120   S2(I)=SSAVE(I)                                                   CREK     205
        ASSIGN 200 TO NEXTOK                                             CREK     206
        ASSIGN 170 TO NEXTNG                                             CREK     207
        GO TO 500                                                        CREK     208
C                                                                        CREK     209
C-----GARBAGE ESTIMATES  (GORDON AND MCBRIDE)                            CREK     210
C                                                                        CREK     211
  170   TK=3800.000                                                      CREK     212
        SM=0.100/FLOAT(NS)                                               NOXXX     6
        DO 171 I=1,NS                                                    CREK     214
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  171 S2(I)=SM                                                          CREK      215
      SM=0.10C                                                          CREK      216
      IF (MODE.EQ.1) ASSIGN 900 TO NEXTOK                               CREK      217
      IF (MODE.EQ.2) ASSIGN 300 TO NEXTOK                               CREK      218
      IF (MODE.GE.3) ASSIGN 200 TO NEXTOK                               CREK      219
      ASSIGN 600 TO NEXTNG                                              CREK      220
      GO TO 500                                                         CREK      221
C                                                                       CREK      222
C**  **  **  **  **  **  **  **  **  **  **  **  CHAPTER 2  **  **  **   CREK      223
C**  **  **  **  **  **  **  **  **  **  **  **  CHAPTER 2  **  **  **   CREK      224
C                                                                       CREK      225
C  ***KINETIC***                                                        CREK      226
C  SECTION FOR KINETIC SOLUTION FROM ADIABATIC EQUILIBRIUM ESTIMATES    CREK      227
C  (MODE 3 AND 4 ONLY)                                                  CREK      228
C                                                                       CREK      229
C-----NEAR-EQUILIBRIUM SOLUTION  (KINETIC WITH EMV=1.00-3 KG/CU M-SEC)  CREK      230
C                                                                       CREK      231
  200 LEQUIL=.FALSE.                                                    CREK      232
      IX=0                                                              CREK      233
      EMV=1.00-3                                                        CREK      234
      XLO=EMV                                                           CREK      235
C-----INCREASE MINOR SPECIES FROM EQUILIBRIUM ESTIMATES                 CREK      236
      DO 201 I=1,NS                                                     CREK      237
      IF (S2(I).LT.SMALL) S2(I)=SMALL                                   CREK      238
  201 CONTINUE                                                          CREK      239
      ASSIGN 230 TO NEXTOK                                              CREK      240
      ASSIGN 210 TO NEXTNG                                              CREK      241
      GO TO 500                                                         CREK      242
C                                                                       CREK      243
C                                                                       CREK      244
C-----FAILURE ON NEAR-EQUIL WITH EMV=XLO, DECREASE EMV BY AN ORDER OF   CREK      245
C-----MAGNITUDE AND ATTEMPT AGAIN, ITERATING THIS WAY UP TO 12 TIMES    CREK      246
C                                                                       CREK      247
  210 EMV=EMV*0.100                                                     CREK      248
      XLO=EMV                                                           CREK      249
      IX=IX+1                                                           CREK      250
      IF (IX.EQ.12) GO TO 610                                           CREK      251
      TK=TSAVE                                                          CREK      252
      DO 211 I=1,NS                                                     CREK      253
  211 S2(I)=SSAVE(I)                                                    CREK      254
      ASSIGN 230 TO NEXTOK                                              CREK      255
      ASSIGN 210 TO NEXTNG                                              CREK      256
      GO TO 500                                                         CREK      257
C                                                                       CREK      258
C                                                                       CREK      259
C-----HAVE NEAR-EQUIL SOLUTION, SO FIRST TRY DIRECTLY TO OBTAIN         CREK      260
C-----REQUIRED SOLUTION AT GIVEN EMV                                    CREK      261
C                                                                       CREK      262
  230 EMV=EMVSAV                                                        CREK      263
      IF (MODE.EQ.3) ASSIGN 900 TO NEXTOK                               CREK      264
      IF (MODE.EQ.4) ASSIGN 300 TO NEXTOK                               CREK      265
      ASSIGN 250 TO NEXTNG                                              CREK      266
      GO TO 500                                                         CREK      267
C                                                                       CREK      268
C  ***UPPER BRANCH MARCHING***                                          CREK      269
C     HAVE A KINETIC SOLUTION BUT AT EMV .LT. EMVSAV.  START AT         CREK      270
C     KNOWN SOLUTION AND INCREASE EMV BY FACTOR TO MOVE TOWARDS         CREK      271
C     A SOLN THERE, IF SUCCESSFUL, REPEAT UNTIL EMVSAV IS REACHED  IF   CREK      272
C     NOT SUCCESSFUL START HALF INTERVAL SEARCHING DESCRIBED BELOW      CREK      273
C                                                                       CREK      274
  250 EMV=XLO*FACTOR                                                    CREK      275
      IF (EMV.GT.EMVSAV) EMV=EMVSAV                                     CREK      276
      XHI=EMV                                                           CREK      277
      IX=0                                                              CREK      278
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      TK=TSAVE                                                          CREK      279
      DO 251 I=1,NS                                                     CREK      280
  251 S2(I)=SSAVE(I)                                                    CREK      281
      ASSIGN 250 TO NEXTOK                                              CREK      282
      IF (EMV.GE.EMVSAV.AND.MODE.EQ.3) ASSIGN 900 TO NEXTOK             CREK      283
      IF (EMV.GE.EMVSAV.AND.MODE.EQ.4) ASSIGN 900 TO NEXTOK             CREK      284
      ASSIGN 270 TO NEXTNG                                              CREK      285
      GO TO 500                                                         CREK      286
C                                                                       CREK      287
C  ***HALF-INTERVAL SEARCHING***                                        CREK      288
C  HAVE SOLUTION AT XLO BUT NOT AT XHI. HENCE START INTERVAL            CREK      289
C  SEARCHING BY SETTING EMV TO THE LOGARITHMIC AVERAGE                  CREK      290
C  IF ITERATING MORE THAN TEN TIMES, TERMINATE.                         CREK      291
C                                                                       CREK      292
  270 IX=IX+1                                                           CREK      293
      TK=TSAVE                                                          CREK      294
      DO 271 I=1,NS                                                     CREK      295
  271 S2(I)=SSAVE(I)                                                    CREK      296
      IF (IX.GT.10) GO TO 620                                           CREK      297
      EMV=DSQRT(XLO*XHI)                                                CREK      298
      XHI=EMV                                                           CREK      299
      ASSIGN 250 TO NEXTOK                                              CREK      300
      ASSIGN 270 TO NEXTNG                                              CREK      301
      GO TO 500                                                         CREK      302
C                                                                       CREK      303
C***   ***   ***   ***   ***   ***   ***   ***   CHAPTER 3   ***   ***  CREK      304
C***   ***   ***   ***   ***   ***   ***   ***   CHAPTER 3   ***   ***  CREK      305
C                                                                       CREK      306
C  ***NON-ADIABATIC***                                                  CREK      307
C  SECTION FOR NON-ADIABATIC SOLUTIONS FROM ADIABATIC ESTIMATES         CREK      308
C  (MODE 2 AND 4 ONLY)                                                  CREK      309
C  TRY DIRECTLY TO OBTAIN NON-ADIABATIC SOLUTION  IF NOT SUCCESSFUL,    CREK      310
C  START HALF-INTERVAL SCALING FROM THE ADIABATIC SOLUTION BY           CREK      311
C  DEFINING A SCALING FACTOR FQ (0.0-1.0) TO MULTIPLY THE NON-ADIABATIC CREK      312
C  TERM (Q) IN THE ENERGY EQUATION IN SPECE                             CREK      313
C                                                                       CREK      314
  300 LADIAB=.FALSE.                                                    CREK      315
      XLO=0.0D0                                                         CREK      316
      XHI=1.0D0                                                         CREK      317
      FQ=1.0D0                                                          CREK      318
      IX=0                                                              CREK      319
  310 ASSIGN 320 TO NEXTOK                                              CREK      320
      ASSIGN 330 TO NEXTNG                                              CREK      321
      GO TO 500                                                         CREK      322
C                                                                       CREK      323
  320 IF (FQ.EQ.1.0D0) GO TO 900                                        CREK      324
      XLO=FQ                                                            CREK      325
      FQ=1.000                                                          CREK      326
      XHI=1.000                                                         CREK      327
      IX=0                                                              CREK      328
      GO TO 310                                                         CREK      329
C                                                                       CREK      330
  330 IX=IX+1                                                           CREK      331
      IF (IX.GT.10) GO TO 340                                           CREK      332
      TK=TSAVE                                                          CREK      333
      DO 331 I=1,NS                                                     CREK      334
  331 S2(I)=SSAVE(I)                                                    CREK      335
      FQ=0.500*(XLO+XHI)                                                CREK      336
      XHI=FQ                                                            CREK      337
      GO TO 310                                                         CREK      338
C                                                                       CREK      339
  340 FQ=1.000                                                          CREK      340
      GO TO 630                                                         CREK      341
C                                                                       CREK      342
```

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C****    ****    ****    ****    ****    ****    CHAPTER 4   ****  ***   CREK      343
C****    ****    ****    ****    ****    ****    CHAPTER 4   ****  ***   CREK      344
C                                                                          CREK      345
C  ***FAILURE EXITS***                                                     CREK      346
C  FAILED EQUIL OR KINETIC SOLN OR EQUIV RATIO OUTSIDE (0.1,10)            CREK      347
C  RETURN ADIABATIC, NON-REACTED MIXTURE PROPERTIES                        CREK      348
  400 SM=0.000                                                             CREK      349
      DO 401 I=1,NS                                                        CREK      350
      S2(I)=S1(I)                                                          CREK      351
      SM=SM+S2(I)                                                          CREK      352
  401 CONTINUE                                                             CREK      353
      TK=1000.000                                                          CREK      354
      XLO=TK                                                               CREK      355
      IHCPS=1                                                              CREK      356
      NS1=1                                                                NOXX       16
      NS2=NS                                                               NOXX       17
      TKINV=1.0D-3                                                         CREK      357
      DO 403 I=1,30                                                        NOXX       18
      CALL HCPS                                                            CREK      359
      HSUM=0.000                                                           CREK      360
      DO 402 K=1,NS                                                        CREK      361
      HSUM=HSUM+HO(K)*S2(K)                                                CREK      362
  402 CONTINUE                                                             CREK      363
      IF(.NOT.LADIAB)HSUM=HSUM+(((Q4*TK+Q3)*TK+Q2)*TK+Q1+Q0*TKINV)/        CREK      364
     1(RGAS*EMW)                                                           CREK      365
      TK=TK*(1.000+0.500*(HSUBO*RGASIN*TKINV-HSUM)/CPSUM)                  NOXX       19
      TKINV=1.000/TK                                                       CREK      367
      XHI=DABS(TK-XLO)                                                     CREK      368
      XLO=TK                                                               CREK      369
      IF (XHI.LT.1.000) GO TO 404                                          CREK      370
  403 CONTINUE                                                             CREK      371
  404 CONTINUE                                                             CREK      375
      IF(.NOT.LADIAB)HSUBO=HSUM*RGAS*TK                                    CREK      376
C                                                                          CREK      377
      GO TO 900                                                            CREK      378
C                                                                          CREK      379
C*****      *****      *****      *****      *****   CHAPTER 5   ***** *   CREK      380
C*****      *****      *****      *****      *****   CHAPTER 5   ***** *   CREK      381
C                                                                          CREK      382
C  ***PROBLEM CELL CALL TO SPECE***                                        CREK      383
C  TAKE THE ESTIMATES GENERATED IN CHAPTERS 1,2 AND ATTEMPT A SOLUTION     CREK      384
C  WITH FULL EQUATIONS. IF SUCCESSFUL, UPDATE THE SAVE ANSWERS WITH THE    CREK      385
C  SOLUTION AND RETURN TO STATEMENT NUMBER NEXTOK.  IF NOT, THE ACTION     CREK      386
C  DEPENDS ON WHETHER AN EQUILOM OR KINETIC SOLN IS SOUGHT.  FAILED        CREK      387
C  EQUIL SOLN, RETURN TO STATEMENT NUMBER NEXTNG, WHILE FAILURE IN A       CREK      388
C  KINETIC SOLN WILL BE FOLLOWED BY AN ATTEMPT WITH LNRG=F ---  RT=0.0     CREK      389
C  AND SAME ESTIMATES.  SETTING RT=0.0 IMPLIES THAT A CHANGE IN TEMP       CREK      390
C  FIELD HAS NO EFFECT ON SPECIES DISTRIBUTION FOR THAT PARTICULAR         CREK      391
C  ITERATION, BUT DOES ALLOW THE SPECIES CHANGES TO INFLUENCE THE TEMP     CREK      392
C  CHANGE ---  PARTIAL DECOUPLING OF THE ENERGY EQUATION.                  CREK      393
C  IF STILL NO GOOD, RETURN TO STATEMENT NUMBER NEXTNG.                    CREK      394
C                                                                          CREK      395
  500 CALL SPECE                                                           CREK      396
      IF (LCONVG) GO TO 540                                                CREK      397
C     SOLUTION FAILED TRY RT=0.0                                           CREK      398
      IF (LNRG) GO TO 520                                                  CREK      399
      LNRG=.TRUE.                                                          CREK      400
  510 GO TO NEXTNG, (100,170,210,250,270,330,600)                          CREK      401
  520 IF (LEQUIL) GO TO 510                                                CREK      402
  530 LNRG=.FALSE.                                                         CREK      403
      GO TO 500                                                            CREK      404
  540 IF (LNRG) GO TO 550                                                  CREK      405
      LNRG=.TRUE.                                                          CREK      406
C                                                                          CREK      407
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C     GO TO 500      **REMOVED PER D.T.PRATT  7/19/78**                    CREK     408
C******IF COMPLEX CASES DO NOT CONVERGE, IT MAY BE NECESSARY TO******      CREK     409
C******RETURN THIS STATEMENT TO THE PROGRAM.                 *********     CREK     410
C                                                                          CREK     411
C                                                                          CREK     412
C-----SOLUTION IS SUCCESSFUL, UPDATE SAVE ANSWERS AND CONTINUE.            CREK     413
C                                                                          CREK     414
  550 TSAVE=TK                                                             CREK     415
      DO 560 I=1,NS                                                        CREK     416
  560 SSAVE(I)=S2(I)                                                       CREK     417
C                                                                          CREK     418
      GO TO NEXTOK, (200,230,250,300,320,900)                              CREK     419
C                                                                          CREK     420
C******       ******       ******       ******       CHAPTER 6    ******  CREK     421
C******       ******       ******       ******       CHAPTER 6    ******  CREK     422
C                                                                          CREK     423
C  ***ERROR MESSAGES***                                                    CREK     424
C                                                                          CREK     425
  600 WRITE(6,601)                                                         CREK     426
  601 FORMAT(1HO,10X,3(4H****),30H FAILURE TO FIND EQUIL SOLN....          CREK     427
     A24HAVG INLET PROPS RETURNED/)                                        CREK     428
      GO TO 650                                                            CREK     429
  610 WRITE(6,611)                                                         CREK     430
  611 FORMAT(1HO,10X,3(4H****),35H FAILURE TO FIND NEAR-EQUIL SOLN....     CREK     431
     A24HAVG INLET PROPS RETURNED/)                                        CREK     432
      GO TO 650                                                            CREK     433
  620 WRITE(6,621)                                                         CREK     434
  621 FORMAT(1HO,10X,3(4H****),37H FAILURE TO OBTAIN KINETIC SOLN AFTER,   CREK     435
     A48H TEN INTERVAL HALVING...AVG INLET PROPS RETURNED/)                CREK     436
      GO TO 650                                                            CREK     437
  630 WRITE(6,631)                                                         CREK     438
  631 FORMAT(1HO,10X,3(4H****),29H NON-ADIABATIC SOLN FAILED....           CREK     439
     A19HADIAB SOLN RETURNED/)                                             CREK     440
      GO TO 670                                                            CREK     441
C                                                                          CREK     442
C-----RESTORE FAILED PROBLEM MODE PRIOR TO RETURN                          CREK     443
C                                                                          CREK     444
  650 IF (MODE.EQ.2) LADIAB=.FALSE.                                        CREK     445
      IF (MODE.EQ.3) LEQUIL=.FALSE.                                        CREK     446
      IF (MODE.EQ.4) LADIAB=.FALSE.                                        CREK     447
      GO TO 400                                                            CREK     448
C                                                                          CREK     449
C-----FAILED NON-ADIABATIC SOLUTION...RETURN ADIABATIC                     CREK     450
C-----EQUIL OR KINETIC SOLUTION                                            CREK     451
C                                                                          CREK     452
  670 TK=TSAVE                                                             CREK     453
      SM=0.000                                                             CREK     454
      DO 671 I=1,NS                                                        CREK     455
      S2(I)=SSAVE(I)                                                       CREK     456
  671 SM=SM+S2(I)                                                          CREK     457
  900 RHOP=PA/(RGAS*TK*SM)                                                 CREK     458
      RETURN                                                               CREK     459
      END                                                                  CREK     460
      SUBROUTINE CALC                                                      CALC       2
C                                                                          CALC       3
      DOUBLE PRECISION AL,BO,CPSUM,EMV,ER,FQ,HSUBO,HSUM,HO,PA,PI,PPLN,     NOXX      20
     1 QQ,Q1,Q2,Q3,Q4,RGAS,RGASIN,RHOP,SM,SMINV,SMW,SSAVE,SQ,S1,S2,TK,     NOXXX      8
     2 TKINV,TLN,Z,SMO                                                     NOXXX      9
      DOUBLE PRECISION BK,BX2,TACT,TACT2,TEN,TEN2,Y1,X2,CEBU               NOXX      21
      DOUBLE PRECISION XCTH,FUT,FST,SSS                                    4STEP    345
      DOUBLE PRECISION X,Y                                                 NOXXX     11
      DOUBLE PRECISION ANO,BIG,BXX,DSUM,EN,HH,HIN,Q,QDRV,RHSN,RHSQ,        NOXXX     12
     1 RN,RT,R1,R2,SS,SUM,S2I,TK1,TK2,TM1,TM2,TM3,TN2,XC,YH                NOXXX     13
      LOGICAL LADIAB,LCONVG,LDEBUG,LEQUIL,LNRG,LREACT,LENER                NOXXX     14
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      DOUBLE PRECISION RLAN,RTURB,PHI                                    NOXX      22
C                                                                        CALC       6
C     THE FOLLOWING DOUBLE PRECISION REQUIRED ONLY FOR IBM MACHINES      CALC       7
      DOUBLE PRECISION A,QTM1                                            CALC       8
C                                                                        CALC       9
      COMMON                                                             CALC      10
     3/CCHEMI/CPSUM,HSUM,FQ,PPLN,RGAS,RGASIN,SMINV,TKINV,TLN,LNRG        NOXX      23
     1/CEQUIL/AL(7,30),ATOM(3,7),RO(7),PI(7)                             CALC      12
     1/CINDEX/IDCO,IDFU,IDO2,IDN2,IDH2O,IDCO2,IDH1,IDH2,IDN1,IDNO,IDNO2  NOXX      24
     1,IDO,IDOH,IHCPS,ILC,ILH,IMAT,ITER,JJ,N1,N2,N3,NA,NGLOB,NGLOBP,     NOXX      25
     2 NLM,NQ,NSM,NS1,NS2,IDCH                                           4STEP     346
     1/CMATRI/X(32),Y(32)                                                NOXX      27
     1/CPARAM/ASUB(30,3),ENV,ER,HSUBO,NDEBUG,NS,PA,QQ,Q1,Q2,Q3,Q4,RHOP,  CALC      16
     1 SN,SNW(30),SMO,S1(30),S2(30),TK,LADIAB,LDEBUG,LEQUIL,LREACT,LENER NOXX      28
     2,EQKIJ,LCONVG                                                      NOXX      29
     1/CREACT/BX(36),BX2(36),ID(6,36),NOOR(36),TACT(36),TACT2(36),       CALC      18
     2 TEN(36),TEN2(36),X1(36),X2(36),CEBU(36)                           NOXX      30
     1/CSPECE/HO(30),SO(30),SSAVE(30),Z(7,2,30)                          NOXX      31
      COMMON/STEP4/PEXP1,PEXP2,PEXP3,PEXP4,ER1,ER2,ER3,ER4,CEBU1,CEBU2,  4STEP     347
     1 CERU3,CEBU4,AEXP1,AEXP2,AEXP3,AEXP4,BEXP1,BEXP2,BEXP3,BEXP4,      4STEP     348
     2 CEXP1,CEXP2,CEXP3,CEXP4,FUT,FST                                   4STEP     349
C                                                                        CALC      21
C*************************************************************************CALC      22
C  THIS SUBROUTINE CONSTRUCTS THE NEWTON-RAPHSON DERIVATIVE MATRIX FOR   CALC      23
C  BOTH KINETIC AND EQUILIBRIUM SOLUTIONS AND SOLVES IT BY PIVOTAL       CALC      24
C  GAUSSIAN REDUCTION.  WHENEVER TEMP IS LESS THAN 1500K, THE REVERSE    CALC      25
C  RATE IS CALCULATED FROM THE FORWARD RATE AND EQUILIBRIUM CONSTANT.    CALC      26
C  PROVISION IS MADE FOR GLOBAL REACTIONS                                CALC      27
C  REFERENCE  CREK    (WASHINGTON STATE UNIVERSITY)  MARCH 1976          CALC      28
C*************************************************************************CALC      29
C                                                                        CALC      30
      DIMENSION A(32,33)                                                 CALC      31
C                                                                        CALC      32
      DATA BIG/46.05100/                                                 CALC      33
C                                                                        CALC      34
      DO 10 I=1,NQ                                                       CALC      35
      X(I)=0.0                                                           NOXX      32
      DO 10 K=1,NA                                                       CALC      36
   10 A(I,K)=0.000                                                       CALC      37
C                                                                        CALC      38
      IHCPS=1                                                            CALC      39
      IF (LEQUIL) IHCPS=2                                                CALC      40
      IF (TK.LT.1500.000) IHCPS=2                                        CALC      41
      NS1=1                                                              NOXX      33
      NS2=NS                                                             NOXX      34
      CALL HCPS                                                          CALC      42
      HIN=HSUBO*RGASIN*TKINV                                             CALC      43
      Q=0.000                                                            CALC      44
      QDRV=0.000                                                         CALC      45
      IF (LADIAB) GO TO 20                                               CALC      46
C-----Q AND QDRV ARE NON-DIMENSIONAL                                     CALC      47
      TM1=FQ/(ENV*RGAS)                                                  CALC      48
      Q=(((Q4*TK+Q3)*TK+Q2)*TK+Q1+QQ*TKINV)*TM1                          CALC      49
      QDRV=(((4.000*Q4*TK+3.000*Q3)*TK+2.000*Q2)*TK+Q1)*TM1              CALC      50
   20 CONTINUE                                                           CALC      51
C                                                                        CALC      52
      IF (LEQUIL) GO TO 300                                              CALC      53
C                                                                        CALC      54
      RHSM=PA*RGASIN*TKINV                                               CALC      55
      RHOP=RHSM*SMINV                                                    CALC      56
      RHSQ=RHOP**2                                                       CALC      57
C                                                                        CALC      58
C* * * * * * * * * * * * * * * * * * * * * * CHAPTER 1 * * * * * * * * CALC      59
C* * * * * * * * * * * * * * * * * * * * * * CHAPTER 1 * * * * * * * * CALC      60
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C                                                                       CALC      61
C  ***GLOBAL REACTION***                                               CALC      62
C  GLOBAL RATE EQUATIONS FOR HYDROCARBON PYROLYSIS...                   CALC      63
C   GLOBAL RATE EXPRESSIONS DUE TO KOLLRACK...                          CALC      64
C    (1)  C12H23 + O2 ---  5 C2H4 + C2H3 + O2                           CALC      65
C    (2)  C12H23 + OH ---  6 C2H4 + O                                   CALC      66
C                                                                       CALC      67
      IF (NGLOR.EQ.0) GO TO 110                                         CALC      68
      IF (TK.LT.560.00) GO TO 110                                       CALC      69
      DO 100 J=1,NGLOR                                                  CALC      70
      I=ID(1,J)                                                         CALC      71
      K=ID(2,J)                                                         CALC      72
      M=ID(4,J)                                                         CALC      73
      N=ID(5,J)                                                         CALC      74
      IF(I.EQ.IDFU.AND.M.EQ.IDCH.AND.N.EQ.IDH2)GO TO 150                4STEP    350
      IF(I.EQ.IDCH.AND.K.EQ.ID02)GO TO 160                              4STEP    351
      IF(I.EQ.IDCO.AND.K.EQ.ID02)GO TO 170                              4STEP    352
      IF(I.EQ.IDH2.AND.K.EQ.ID02)GO TO 180                              4STEP    353
      IF(M.EQ.IDCO.AND.N.EQ.IDH2) GO TO 105                             CALC      75
      IF(N.EQ.IDCO.AND.N.EQ.IDH20)GO TO 111                             NOXX      35
      IF(I.EQ.IDCO.AND.K.EQ.ID02)GO TO 121                              NOXX      36
      TK1=TACT(J)*TKINV                                                 CALC      76
      TM2=TK1-TEN(J)*TLN-BX(J)                                          CALC      77
      IF (DABS(TM2).GT.BIG) GO TO 100                                   CALC      78
      R1=DEXP(-TM2)                                                     CALC      79
C                                                                       CALC      80
C-----PROVISION FOR CONTACT INDEX                                       CALC      81
      R1=K1(J)*R1                                                       CALC      82
      R1=R1*S2(I)*RHSQ*S2(K)                                            CALC      83
      RT=R1*(TEN(J)+TK1-2.00)                                           CALC      84
      RN=R1*2.00                                                        CALC      85
C-----A(ANY,M)=A(ANY,N)=0 BECAUSE NO REVERSE REACTION ASSUMED           CALC      86
      A(I,I)=A(I,I)+R1                                                  CALC      87
      A(I,K)=A(I,K)+R1                                                  CALC      88
      A(I,NA)=A(I,NA)-R1                                                CALC      89
      A(I,NSM)=A(I,NSM)-RN                                              CALC      90
      A(I,NQ)=A(I,NQ)+RT                                                CALC      91
      A(N,I)=A(N,I)-R1                                                  CALC      92
      A(N,K)=A(N,K)-R1                                                  CALC      93
      A(N,NA)=A(N,NA)+R1                                                CALC      94
      A(N,NSM)=A(N,NSM)+RN                                              CALC      95
      A(N,NQ)=A(N,NQ)-RT                                                CALC      96
      ANO=5.00                                                          CALC      97
      IF (J.EQ.1) GO TO 101                                             CALC      98
      A(K,I)=A(K,I)+R1                                                  CALC      99
      A(K,K)=A(K,K)+R1                                                  CALC     100
      A(K,NA)=A(K,NA)-R1                                                CALC     101
      A(K,NSM)=A(K,NSM)-RN                                              CALC     102
      A(K,NQ)=A(K,NQ)+RT                                                CALC     103
      ANO=6.00                                                          CALC     104
  101 CONTINUE                                                          CALC     105
      R1=R1*ANO                                                         CALC     106
      RN=RN*ANO                                                         CALC     107
      RT=RT*ANO                                                         CALC     108
      A(M,I)=A(M,I)-R1                                                  CALC     109
      A(M,K)=A(M,K)-R1                                                  CALC     110
      A(M,NA)=A(M,NA)+R1                                                CALC     111
      A(M,NSM)=A(M,NSM)+RN                                              CALC     112
      A(M,NQ)=A(M,NQ)-RT                                                CALC     113
      GO TO 200                                                         CALC     114
  105 CONTINUE                                                          CALC     115
C  ***GLOBAL REACTION***                                                CALC     116
C  GLOBAL RATE EQUATIONS FOR HYDROCARBON PYROLYSIS...                   CALC     117
C  GLOBAL RATE EXPRESSION DUE TO BOELMAN AND FORTUNE                    CALC     118
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C      CHHY + (X/2) O2 ----  X CO + (Y/2) H2                          CALC      119
C                                                                     CALC      120
       XC=AL(ILC,I)                                                   CALC      121
       YH=AL(ILH,I)                                                   NOXXX      15
       TK1=TACT(J)*TKINV                                              CALC      123
       TM2=TK1-RX(J)-(0.3*PPLN)                                       CALC      124
       IF(TEN(J).NE.0.)TM2=TM2-TEN(J)*TLN                             CALC      125
       IF(DABS(TM2).GT.BIG)GO TO 100                                  CALC      126
       R1=DEXP(-TM2)                                                  CALC      127
C                                                                     CALC      128
C-----PROVISION FOR CONTACT INDEX                                     CALC      129
       R1=X1(J)*R1                                                    CALC      130
       R1=R1*(RHOP*S2(K))*DSQRT(RHOP*S2(I))                           CALC      131
       TM1=R1*0.5                                                     CALC      132
       A(I,I)=A(I,I)+TM1                                              CALC      133
       A(I,K)=A(I,K)+R1                                               CALC      134
       A(K,I)=A(K,I)+R1*XC*0.25                                       CALC      135
       A(K,K)=A(K,K)+TM1*XC                                           CALC      136
       A(M,I)=A(M,I)-TM1*XC                                           CALC      137
       A(M,K)=A(M,K)-R1*XC                                            CALC      138
       A(N,I)=A(N,I)-R1*YH*0.25                                       CALC      139
       A(N,K)=A(N,K)-TM1*YH                                           CALC      140
C-----A(ANY,M)=A(ANY,N)=0 BECAUSE NO REVERSE REACTION ASSUMED          CALC      141
       RN=R1*1.5                                                      CALC      142
       A(I,NSM)=A(I,NSM)-RN                                           CALC      143
       A(K,NSM)=A(K,NSM)-RN*XC*0.5                                    CALC      144
       A(M,NSM)=A(M,NSM)+RN*XC                                        CALC      145
       A(N,NSM)=A(N,NSM)+RN*YH*0.5                                    CALC      146
       A(I,NA)=A(I,NA)-R1                                             CALC      147
       A(K,NA)=A(K,NA)-R1*XC*0.5                                      CALC      148
       A(M,NA)=A(M,NA)+R1*XC                                          CALC      149
       A(N,NA)=A(N,NA)+R1*YH*0.5                                      CALC      150
       IF (.NOT.LNRG) GO TO 100                                       CALC      151
       RT=R1*(TK1+TEN(J)-1.5)                                         CALC      152
       A(I,NQ)=A(I,NQ)+RT                                             CALC      153
       A(K,NQ)=A(K,NQ)+RT*XC*0.5                                      CALC      154
       A(M,NQ)=A(M,NQ)-RT*XC                                          CALC      155
       A(N,NQ)=A(N,NQ)-RT*YH*0.5                                      CALC      156
       GO TO 100                                                      NOXX       37
  111 CONTINUE                                                        NOXX       38
C  ***GLOBAL REACTION***                                              NOXX       39
C  GLOBAL RATE EQUATIONS FOR 2-STEP REACTION.                         NOXX       40
C  FIRST STEP   CXHY+(X/2+Y/4)O2 --- XCO+(Y/2)H2O                     NOXX       41
C                                                                     NOXX       42
       XC=AL(ILC,I)                                                   NOXX       43
       YH=AL(ILH,I)                                                   NOXX       44
       TK1=TACT(J)*TKINV                                              NOXX       45
       TM2=TK1-RX(J)-TEN(J)*TLN                                       NOXX       46
       IF(DABS(TM2).GT.BIG)GO TO 100                                  NOXX       47
       R1=DEXP(-TM2)                                                  NOXX       48
C                                                                     NOXX       49
C-----PROVISION FOR CONTACT INDEX.                                    NOXX       50
       R1=X1(J)*R1                                                    NOXX       51
       R1=R1*(RHOP*S2(K))*DSQRT(RHOP*S2(I))                           NOXX       52
       RLAM=R1                                                        NOXX       53
       PHI=DMIN1(S2(I),S2(K)/(XC+0.25*YH))                            NOXX       54
       RTURB=CTAU(J)*RHOP*PHI*EOKTJ                                   NOXX       55
       IF(RLAM.LT.RTURB)GO TO 130                                     NOXX       56
       R1=RTURB                                                       NOXX       57
       FN=1.000                                                       NOXX       58
       IF(S2(K)/(XC+0.25*YH).LT.S2(I))GO TO 131                       NOXX       59
       R11=RTURB                                                      NOXX       60
       R1K=0.0                                                        NOXX       61
       GO TO 132                                                      NOXX       62
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  131 R1I=0.0                                                          NOXX   63
      R1K=RTURB                                                        NOXX   64
      GO TO 132                                                        NOXX   65
  130 R1I=0.500*RLAM                                                   NOXX   66
      R1K=RLAM                                                         NOXX   67
      R1=RLAM                                                          NOXX   68
      EN=1.500                                                         NOXX   69
  132 CONTINUE                                                         NOXX   70
      A(I,I)=A(I,I)+R1I                                                NOXX   71
      A(I,K)=A(I,K)+R1K                                                NOXX   72
      A(K,I)=A(K,I)+R1I*0.5*(XC+0.5*YH)                                NOXX   73
      A(K,K)=A(K,K)+0.5*R1K*(XC+0.5*YH)                                NOXX   74
      A(M,I)=A(M,I)-R1I*XC                                             NOXX   75
      A(M,K)=A(M,K)-R1K*XC                                             NOXX   76
      A(N,I)=A(N,I)-R1I*YH*0.5                                         NOXX   77
      A(N,K)=A(N,K)-0.5*R1K*YH                                         NOXX   78
C-----A(ANY,M)=A(ANY,N)=0  BECAUSE NO REVERSE REACTION ASSUMED.        NOXX   79
      RN=R1*EN                                                         NOXX   80
      A(I,NSM)=A(I,NSM)-RN                                             NOXX   81
      A(K,NSM)=A(K,NSM)-RN*0.5*(XC+0.5*YH)                             NOXX   82
      A(M,NSM)=A(M,NSM)+RN*XC                                          NOXX   83
      A(N,NSM)=A(N,NSM)+RN*YH*0.5                                      NOXX   84
      A(I,NA)=A(I,NA)-R1                                               NOXX   85
      A(K,NA)=A(K,NA)-R1*0.5*(XC+0.5*YH)                               NOXX   86
      A(M,NA)=A(M,NA)+R1*XC                                            NOXX   87
      A(N,NA)=A(N,NA)+R1*YH*0.5                                        NOXX   88
      IF(.NOT.LNRG)GO TO 100                                           NOXX   89
      IF(RTURB.LT.RLAM)GO TO 100                                       NOXX   90
      RT=R1*(TK1*TEN(J)-1.5)                                           NOXX   91
      A(I,NQ)=A(I,NQ)+RT                                               NOXX   92
      A(K,NQ)=A(K,NQ)+RT*0.5*(XC+0.5*YH)                               NOXX   93
      A(M,NQ)=A(M,NQ)-RT*XC                                            NOXX   94
      A(N,NQ)=A(N,NQ)-RT*YH*0.5                                        NOXX   95
      GO TO 100                                                        NOXX   96
  121 CONTINUE                                                         NOXX   97
C   ***GLOBAL REACTION***                                              NOXX   98
C   GLOBAL RATE EQUATIONS FOR 2-STEP REACTION.                         NOXX   99
C   SECOND STEP    CO+(1/2)O2 --- CO2                                  NOXX  100
C                                                                      NOXX  101
      TK1=TACT(J)*TKINV                                                NOXX  102
      TM2=TK1-BX(J)-TEN(J)*TLN                                         NOXX  103
      IF(DABS(TM2).GT.BIG)GO TO 100                                    NOXX  104
      R1=DEXP(-TM2)                                                    NOXX  105
C                                                                      NOXX  106
C-----PROVISION FOR CONTACT INDEX.                                     NOXX  107
      R1=X1(J)*R1                                                      NOXX  108
      R1=R1*RHSQ*S2(K)*S2(I)                                           NOXX  109
      RLAM=R1                                                          NOXX  110
      PHI=DMIN1(2.*S2(K),S2(I))                                        NOXX  111
      RTURB=CERU(J)*RHOP*PHI*EDKIJ                                     NOXX  112
      IF(RLAM.LT.RTURB)GO TO 140                                       NOXX  113
      R1=RTURB                                                         NOXX  114
      EN=1.000                                                         NOXX  115
      IF(2.*S2(K).LT.S2(I))GO TO 141                                   NOXX  116
      R1I=RTURB                                                        NOXX  117
      R1K=0.0                                                          NOXX  118
      GO TO 142                                                        NOXX  119
  141 R1I=0.0                                                          NOXX  120
      R1K=RTURB                                                        NOXX  121
      GO TO 142                                                        NOXX  122
  140 R1I=RLAM                                                         NOXX  123
      R1K=RLAM                                                         NOXX  124
      R1=RLAM                                                          NOXX  125
      EN=2.000                                                         NOXX  126
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  142 CONTINUE                                                          NOXX      127
      A(I,I)=A(I,I)+R1I                                                 NOXX      128
      A(I,K)=A(I,K)+R1K                                                 NOXX      129
      A(K,I)=A(K,I)+0.5*R1I                                             NOXX      130
      A(K,K)=A(K,K)+0.5*R1K                                             NOXX      131
      A(M,I)=A(M,I)-R1I                                                 NOXX      132
      A(M,K)=A(M,K)-R1K                                                 NOXX      133
C-----A(ANY,M)=A(ANY,N)=0  BECAUSE NO REVERSE REACTION ASSUMED.         NOXX      134
      RN=R1*EN                                                          NOXX      135
      A(I,NSM)=A(I,NSM)-RN                                              NOXX      136
      A(K,NSM)=A(K,NSM)-RN*0.5                                          NOXX      137
      A(M,NSM)=A(M,NSM)+RN                                              NOXX      138
      A(I,NA)=A(I,NA)-R1                                                NOXX      139
      A(K,NA)=A(K,NA)-R1*0.5                                            NOXX      140
      A(M,NA)=A(M,NA)+R1                                                NOXX      141
      IF(.NOT.LNRG)GO TO 100                                            NOXX      142
      IF(RTURB.LT.RLAM)GO TO 100                                        NOXX      143
      RT=R1*(TK1+TEN(J)-2.0)                                            NOXX      144
      A(I,NQ)=A(I,NQ)+RT                                                NOXX      145
      A(K,NQ)=A(K,NQ)+RT*0.5                                            NOXX      146
      A(M,NQ)=A(M,NQ)-RT                                                NOXX      147
      GO TO 100                                                         4STEP     354
  150 CONTINUE                                                          4STEP     355
C  ***GLOBAL REACTION***                                                4STEP     356
C  GLOBAL RATE EQUATIONS FOR 4-STEP REACTION.                           4STEP     357
C  FIRST STEP   CXHY --- CXHY-2+H2                                      4STEP     358
C                                                                       4STEP     359
      XC=AL(ILC,I)                                                      4STEP     360
      YH=AL(ILH,I)                                                      4STEP     361
      TACT(J)=ER1                                                       4STEP     362
      TEN(J)=0.000                                                      4STEP     363
      CEBU(J)=CEBU1                                                     4STEP     364
      AX(J)=AEXP1                                                       4STEP     365
      TK1=TACT(J)*TKINV                                                 4STEP     366
      TM2=TK1-AX(J)-TEN(J)*TLN                                          4STEP     367
      IF(DABS(TM2).GT.BIG)GO TO 100                                     4STEP     368
      R1=DEXP(-TM2)                                                     4STEP     369
C                                                                       4STEP     370
C-----PROVISION FOR CONTACT INDEX.                                      4STEP     371
      R1=X1(J)*R1                                                       4STEP     372
      R1=R1*((RHOP*S2(IDFU))**AEXP1)*((RHOP*S2(IDO2))**BEXP1)           4STEP     373
     1*((RHOP*S2(IDCH))**CEXP1)                                         4STEP     374
      RLAM=R1                                                           4STEP     375
      PHI=S2(I)                                                         4STEP     376
      RTURB=CEBU(J)*RHOP*PHI*EDKIJ                                      4STEP     377
      IF(RLAM.LT.RTURB)GO TO 151                                        4STEP     378
      R1=RTURB                                                          4STEP     379
      EN=1.000                                                          4STEP     380
      R1I=RTURB                                                         4STEP     381
      R1M=0.0                                                           4STEP     382
      R1O2=0.0                                                          4STEP     383
      GO TO 152                                                         4STEP     384
  151 R1I=AEXP1*RLAM                                                    4STEP     385
      R1O2=BEXP1*RLAM                                                   4STEP     386
      R1M=CEXP1*RLAM                                                    4STEP     387
      R1=RLAM                                                           4STEP     388
      EN=AEXP1+BEXP1+CEXP1                                              4STEP     389
  152 A(I,I)=A(I,I)+R1I                                                 4STEP     390
      A(I,M)=A(I,M)+R1M                                                 4STEP     391
      A(I,IO2)=A(I,IO2)+R1O2                                            4STEP     392
      A(M,I)=A(M,I)-R1I                                                 4STEP     393
      A(M,M)=A(M,M)-R1M                                                 4STEP     394
      A(M,IO2)=A(M,IO2)-R1O2                                            4STEP     395
      A(N,I)=A(N,I)-R1I                                                 4STEP     396
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      A(M,M)=A(M,M)-R1M                                                 4STEP   397
      A(M,IDO2)=A(M,IDO2)-R1O2                                          4STEP   398
      RN=R1*FN                                                          4STEP   399
      A(I,NSM)=A(I,NSM)-RN                                              4STEP   400
      A(M,NSM)=A(M,NSM)+RN                                              4STEP   401
      A(N,NSM)=A(N,NSM)+RN                                              4STEP   402
      A(I,NA)=A(I,NA)-R1                                                4STEP   403
      A(M,NA)=A(M,NA)+R1                                                4STEP   404
      A(N,NA)=A(N,NA)+R1                                                4STEP   405
      IF(.NOT.LNRG)GO TO 100                                            4STEP   406
      IF(RTURB.LT.RLAM)GO TO 100                                        4STEP   407
      RT=R1*(TK1+TEN(J)-EN)                                             4STEP   408
      A(I,NQ)=A(I,NQ)+RT                                                4STEP   409
      A(M,NQ)=A(M,NQ)-RT                                                4STEP   410
      A(N,NQ)=A(N,NQ)-RT                                                4STEP   411
      GO TO 100                                                         4STEP   412
  160 CONTINUE                                                          4STEP   413
C  ***GLOBAL REACTION***                                                4STEP   414
C  GLOBAL RATE EQUATIONS FOR 4-STEP REACTION.                           4STEP   415
C  SECOND STEP    CXHY-2+(X/2)O2 --- XCO+((Y-2)/2)H2                    4STEP   416
C                                                                       4STEP   417
      XC=AL(ILC,IDFU)                                                   4STEP   418
      YH=AL(ILH,IDFU)                                                   4STEP   419
      XCYH=XC+0.2500*(YH-2.0D0)                                         4STEP   420
      TACT(J)=ER2                                                       4STEP   421
      TEN(J)=0.0D0                                                      4STEP   422
      CERU(J)=CERU2                                                     4STEP   423
      RX(J)=REXP2                                                       4STEP   424
      TK1=TACT(J)*TKINV                                                 4STEP   425
      TM2=TK1-RX(J)-TEN(J)*TLN                                          4STEP   426
      IF(DABS(TM2).GT.BIG)GO TO 100                                     4STEP   427
      R1=DEXP(-TM2)                                                     4STEP   428
C                                                                       4STEP   429
C-----*PROVISION FOR CONTACT INDEX.                                     4STEP   430
      R1=K1(J)*R1                                                       4STEP   431
      R1=R1*((RHOP*S2(IDCH))**AEXP2)*((RHOP*S2(IDO2))**BEXP2)           4STEP   432
     1*((RHOP*S2(IDFU)+1.D-30)**CEXP2)                                  4STEP   433
      RLAM=R1                                                           4STEP   434
      PHI=DMIN1(S2(IDCH),S2(IDO2)/XCYH)                                 4STEP   435
      RTURB=CERU(J)*RHOP*PHI*EDKIJ                                      4STEP   436
      IF(RLAM.LT.RTURB)GO TO 161                                        4STEP   437
      R1=RTURB                                                          4STEP   438
      R1FU=0.0                                                          4STEP   439
      EN=1.0D0                                                          4STEP   440
      IF(S2(IDO2)/XCYH.LT.S2(IDCH))GO TO 162                            4STEP   441
      R1I=RTURB                                                         4STEP   442
      R1K=0.0                                                           4STEP   443
      GO TO 163                                                         4STEP   444
  162 R1I=0.0                                                           4STEP   445
      R1K=RTURB                                                         4STEP   446
      GO TO 163                                                         4STEP   447
  161 R1I=AEXP2*RLAM                                                    4STEP   448
      R1K=BEXP2*RLAM                                                    4STEP   449
      R1FU=CEXP2*RLAM                                                   4STEP   450
      R1=RLAM                                                           4STEP   451
      EN=AEXP2+BEXP2+CEXP2                                              4STEP   452
  163 A(I,I)=A(I,I)+R1I                                                 4STEP   453
      A(I,K)=A(I,K)+R1K                                                 4STEP   454
      A(I,IDFU)=A(I,IDFU)+R1FU                                          4STEP   455
      A(K,I)=A(K,I)+R1I*0.5D0*XC                                        4STEP   456
      A(K,K)=A(K,K)+R1K*0.5D0*XC                                        4STEP   457
      A(K,IDFU)=A(K,IDFU)+R1FU*0.5D0*XC                                 4STEP   458
      A(M,I)=A(M,I)-R1I*XC                                              4STEP   459
      A(M,K)=A(M,K)-R1K*XC                                              4STEP   460
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      A(M,IDFU)=A(M,IDFU)-R1FU*XC                                       4STEP   461
      A(N,I)=A(N,I)-R1I*(YH-2.000)*0.500                                4STEP   462
      A(N,K)=A(N,K)-R1K*(YH-2.000)*0.500                                4STEP   463
      A(N,IDFU)=A(N,IDFU)-R1FU*(YH-2.000)*0.500                         4STEP   464
      RN=R1*EN                                                          4STEP   465
      A(I,NSM)=A(I,NSM)-RN                                              4STEP   466
      A(K,NSM)=A(K,NSM)-RN*0.500*XC                                     4STEP   467
      A(M,NSM)=A(M,NSM)+RN*XC                                           4STEP   468
      A(N,NSM)=A(N,NSM)+RN*(YH-2.000)*0.500                             4STEP   469
      A(I,NA)=A(I,NA)-R1                                                4STEP   470
      A(K,NA)=A(K,NA)-R1*0.500*XC                                       4STEP   471
      A(M,NA)=A(M,NA)+R1*XC                                             4STEP   472
      A(N,NA)=A(N,NA)+R1*(YH-2.000)*0.500                               4STEP   473
      IF(.NOT.LNRG)GO TO 100                                            4STEP   474
      IF(RTURB.LT.RLAM)GO TO 100                                        4STEP   475
      RT=R1*(TK1+TEN(J)-EN)                                             4STEP   476
      A(I,NQ)=A(I,NQ)+RT                                                4STEP   477
      A(K,NQ)=A(K,NQ)+RT*0.500*XC                                       4STEP   478
      A(M,NQ)=A(M,NQ)-RT*XC                                             4STEP   479
      A(N,NQ)=A(N,NQ)-RT*(YH-2.000)*0.500                               4STEP   480
      GO TO 100                                                         4STEP   481
  170 CONTINUE                                                          4STEP   482
C   ***GLOBAL REACTION***                                               4STEP   483
C   GLOBAL RATE EQUATIONS FOR 4-STEP REACTION.                          4STEP   484
C   THIRD STEP   CO+(1/2)O2 --- CO2                                     4STEP   485
C                                                                       4STEP   486
      TACT(J)=ER3                                                       4STEP   487
      TEN(J)=0.000                                                      4STEP   488
      CERU(J)=CERU3                                                     4STEP   489
      RX(J)=REXP3                                                       4STEP   490
      TK1=TACT(J)*TKINV                                                 4STEP   491
      TM2=TK1-RX(J)-TEN(J)*TLN                                          4STEP   492
      IF(DABS(TM2).GT.BIG)GO TO 100                                     4STEP   493
      R1=DEXP1-TM2)                                                     4STEP   494
C                                                                       4STEP   495
C-----PROVISION FOR CONTACT INDEX.                                      4STEP   496
      R1=X1(J)*R1                                                       4STEP   497
      SSS=7.9300*DEXP(-2.4800*FUT*(1.000-FST)/(FST*(1.000-FUT)))        4STEP   498
      SSS=DMIN1(1.000,SSS)                                              4STEP   499
      R1=R1*((RHOP*S2(IDCO))**AEXP3)*((RHOP*S2(IDO2))**BEXP3)           4STEP   500
     1*((RHOP*S2(IDH2O))**CEXP3)*SSS                                    4STEP   501
      RLAM=R1                                                           4STEP   502
      PHI=DMIN1(2.000*S2(K),S2(I))                                      4STEP   503
      RTURB=CERU(J)*RHO**PHI*EDKIJ                                      4STEP   504
      IF(RLAM.LT.RTURB)GO TO 171                                        4STEP   505
      R1=RTURB                                                          4STEP   506
      R1H2O=0.0                                                         4STEP   507
      EN=1.000                                                          4STEP   508
      IF(2.000*S2(K).LT.S2(I))GO TO 172                                 4STEP   509
      R1I=RTURB                                                         4STEP   510
      R1K=0.0                                                           4STEP   511
      GO TO 173                                                         4STEP   512
  172 R1I=0.0                                                           4STEP   513
      R1K=RTURB                                                         4STEP   514
      GO TO 173                                                         4STEP   515
  171 R1I=AEXP3*RLAM                                                    4STEP   516
      R1K=BEXP3*RLAM                                                    4STEP   517
      R1H2O=CEXP3*RLAM                                                  4STEP   518
      R1=RLAM                                                           4STEP   519
      EN=AEXP3+BEXP3+CEXP3                                              4STEP   520
  173 A(I,I)=A(I,I)+R1I                                                 4STEP   521
      A(I,K)=A(I,K)+R1K                                                 4STEP   522
      A(I,IDH2O)=A(I,IDH2O)+R1H2O                                       4STEP   523
      A(K,I)=A(K,I)+R1I*0.500                                           4STEP   524
```

```
      A(K,K)=A(K,K)+R1K*0.5D0                                          4STEP     525
      A(K,IDH2O)=A(K,IDH2O)+R1H2O*0.5D0                                4STEP     526
      A(M,I)=A(M,I)-R1I                                                4STEP     527
      A(M,K)=A(M,K)-R1K                                                4STEP     528
      A(M,IDH2O)=A(M,IDH2O)-R1H2O                                      4STEP     529
      RN=R1*EN                                                         4STEP     530
      A(I,NSM)=A(I,NSM)-RN                                             4STEP     531
      A(K,NSM)=A(K,NSM)-RN*0.5D0                                       4STEP     532
      A(M,NSM)=A(M,NSM)+RN                                             4STEP     533
      A(I,NA)=A(I,NA)-R1                                               4STEP     534
      A(K,NA)=A(K,NA)-R1*0.5D0                                         4STEP     535
      A(M,NA)=A(M,NA)+R1                                               4STEP     536
      IF(.NOT.LNRG)GO TO 100                                           4STEP     537
      IF(RTURB.LT.RLAM)GO TO 100                                       4STEP     538
      RT=R1*(TK1+TEN(J)-EN)                                            4STEP     539
      A(I,NQ)=A(I,NQ)+RT                                               4STEP     540
      A(K,NQ)=A(K,NQ)+RT*0.5D0                                         4STEP     541
      A(M,NQ)=A(M,NQ)-RT                                               4STEP     542
      GO TO 100                                                        4STEP     543
  100 CONTINUE                                                         4STEP     544
C  ***GLOBAL REACTION***                                               4STEP     545
C  GLOBAL RATE EQUATIONS FOR 4-STEP REACTION.                          4STEP     546
C  FOURTH STEP   H2+(1/2)O2 --- H2O                                    4STEP     547
C                                                                      4STEP     548
      TACT(J)=ER4                                                      4STEP     549
      TEN(J)=0.0D0                                                     4STEP     550
      CEBU(J)=CEBU4                                                    4STEP     551
      RX(J)=REXP4                                                      4STEP     552
      TK1=TACT(J)*TKINV                                                4STEP     553
      TM2=TK1-RX(J)-TEN(J)*TLN                                         4STEP     554
      IF(DABS(TM2).GT.RIG)GO TO 100                                    4STEP     555
      R1=DEXP(-TM2)                                                    4STEP     556
C                                                                      4STEP     557
C-----PROVISION FOR CONTACT INDEX.                                     4STEP     558
      R1=V1(J)*R1                                                      4STEP     559
      R1=R1*((RHOP*S2(IDH2))**AEXP4)*((RHOP*S2(IDO2))**BEXP4)          4STEP     560
     1*((RHOP*S2(IDCH)+1.D-30)**CEXP4)                                 4STEP     561
      RLAM=R1                                                          4STEP     562
      PHI=DMIN1(2.0D0*S2(K),S2(I))                                     4STEP     563
      RTURB=CEBU(J)*RHLP*PHI*EDKIJ                                     4STEP     564
      IF(RLAM.LT.RTURB)GO TO 101                                       4STEP     565
      R1=RTURB                                                         4STEP     566
      R1CH=0.0                                                         4STEP     567
      EN=1.0D0                                                         4STEP     568
      IF(2.0D0*S2(K).LT.S2(I))GO TO 102                                4STEP     569
      R1I=RTURB                                                        4STEP     570
      R1K=0.0                                                          4STEP     571
      GO TO 103                                                        4STEP     572
  102 R1I=0.0                                                          4STEP     573
      R1K=RTURB                                                        4STEP     574
      GO TO 103                                                        4STEP     575
  101 R1I=AEXP4*RLAM                                                   4STEP     576
      R1K=BEXP4*RLAM                                                   4STEP     577
      R1CH=CEXP4*RLAM                                                  4STEP     578
      EN=AEXP4+BEXP4+CEXP4                                             4STEP     579
  103 A(I,I)=A(I,I)+R1I                                                4STEP     580
      A(I,K)=A(I,K)+R1K                                                4STEP     581
      A(I,IDCH)=A(I,IDCH)+R1CH                                         4STEP     582
      A(K,I)=A(K,I)+R1I*0.5D0                                          4STEP     583
      A(K,K)=A(K,K)+R1K*0.5D0                                          4STEP     584
      A(K,IDCH)=A(K,IDCH)+R1CH*0.5D0                                   4STEP     585
      A(M,I)=A(M,I)-R1I                                                4STEP     586
      A(M,K)=A(M,K)-R1K                                                4STEP     587
      A(M,IDCH)=A(M,IDCH)-R1CH                                         4STEP     588
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```
      RN=R1*FN                                                          4STEP   589
      A(I,NSM)=A(I,NSM)-RN                                              4STEP   590
      A(K,NSM)=A(K,NSM)-RN*0.500                                        4STEP   591
      A(M,NSM)=A(M,NSM)+RN                                              4STEP   592
      A(I,NA)=A(I,NA)-R1                                                4STEP   593
      A(K,NA)=A(K,NA)-R1*0.500                                          4STEP   594
      A(M,NA)=A(M,NA)+R1                                                4STEP   595
      IF(.NOT.LNRG)GO TO 100                                            4STEP   596
      IF(RTURB.LT.RLAM)GO TO 100                                        4STEP   597
      RT=R1*(TK1+TEN(J)-EN)                                             4STEP   598
      A(I,NQ)=A(I,NQ)+RT                                                4STEP   599
      A(K,NQ)=A(K,NQ)+RT*0.500                                          4STEP   600
      A(M,NQ)=A(M,NQ)-RT                                                4STEP   601
  100 CONTINUE                                                          CALC    157
C                                                                       CALC    158
  110 CONTINUE                                                          CALC    159
      IF(NGLOBP.GT.JJ)GO TO 271                                         4STEP   602
C                                                                       CALC    160
      DO 270 J=NGLOBP,JJ                                                CALC    161
C                                                                       CALC    162
C**  **  **  **  **  **  **  **  **  **  **  **  **  CHAPTER 2  **  **  **  CALC    163
C**  **  **  **  **  **  **  **  **  **  **  **  **  CHAPTER 2  **  **  **  CALC    164
C                                                                       CALC    165
C  ***REACTION RATES***                                                 CALC    166
C  CALCULATE FORWARD AND REVERSE RATES R1 AND R2                        CALC    167
C  THREE TYPES OF REACTIONS                                             CALC    168
C                                                                       CALC    169
C     MODE 1 ... A + B (+C) ---  D + E (+F)                             CALC    170
C     MODE 2 ... AB + M ---  A + B + M                                  CALC    171
C     MODE 3 ... A + B + M ---  AB + M                                  CALC    172
C                                                                       CALC    173
      I=ID(1,J)                                                         CALC    174
      K=ID(2,J)                                                         CALC    175
      KK=ID(3,J)                                                        CALC    176
      M=ID(4,J)                                                         CALC    177
      N=ID(5,J)                                                         CALC    178
      NN=ID(6,J)                                                        CALC    179
      MODE=MODR(J)                                                      CALC    180
C                                                                       CALC    181
      R1=0.000                                                          CALC    182
      R2=0.000                                                          CALC    183
      TM1=0.000                                                         CALC    184
      TM2=0.000                                                         CALC    185
      RN=0.000                                                          CALC    186
      RT=0.000                                                          CALC    187
      R1I=0.0                                                           NOXX    148
      R1K=0.0                                                           NOXX    149
      R1KK=0.0                                                          NOXX    150
      R2M=0.0                                                           NOXX    151
      R2N=0.0                                                           NOXX    152
      R2NN=0.0                                                          NOXX    153
C                                                                       CALC    188
      TK1=TACT(J)*TKINV                                                 CALC    189
      TM2=TK1-BX(J)                                                     CALC    190
      IF (TEN(J).NE.0.00) TM2=TM2-TEN(J)*TLN                            CALC    191
      IF (DABS(TM2).GT.BIG) GO TO 205                                   CALC    192
      R1=DEXP(-TM2)                                                     CALC    193
C-----PROVISION FOR CONTACT INDEX                                       CALC    194
      R1=R1*X1(J)                                                       CALC    195
      IF (MODE-2) 200,201,202                                           CALC    196
  200 R1=R1*S2(I)*RHSQ*S2(K)                                            CALC    197
      RLAM=R1                                                           NOXX    154
      PHI=DMIN1(S2(K),S2(I))                                            NOXX    155
      RTURB=CERU(J)*RHOP**PHI*EDKIJ                                     NOXX    156
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      IF(RLAM.LT.RTURB)GO TO 291                                        NOXX    157
      R1=RTURB                                                          NOXX    158
      EN=1.0D0                                                          NOXX    159
      IF(S2(K).LT.S2(I))GO TO 292                                       NOXX    160
      R1I=RTURB                                                         NOXX    161
      R1K=0.0                                                           NOXX    162
      GO TO 293                                                         NOXX    163
  292 R1I=0.0                                                           NOXX    164
      R1K=RTURB                                                         NOXX    165
      GO TO 293                                                         NOXX    166
  291 R1I=RLAM                                                          NOXX    167
      R1K=RLAM                                                          NOXX    168
      R1=RLAM                                                           NOXX    169
      EN=2.0D0                                                          CALC    198
  293 CONTINUE                                                          NOXX    170
      IF(KK.EQ.0) GO TO 290                                             CALC    199
      RLAM=RLAM*RHOP*S2(KK)                                             NOXX    171
      PHI=DMIN1(PHI,S2(KK))                                             NOXX    172
      RTURB=CEBU(J)*RHOP*PHI*EDKIJ                                      NOXX    173
      IF(RLAM.LT.RTURB)GO TO 294                                        NOXX    174
      EN=1.0D0                                                          NOXX    175
      R1=RTURB                                                          NOXX    176
      IF(S2(K).LT.S2(I))GO TO 295                                       NOXX    177
      IF(S2(I).LT.S2(KK))GO TO 296                                      NOXX    178
      GO TO 298                                                         NOXX    179
  295 IF(S2(K).LT.S2(KK))GO TO 297                                      NOXX    180
  298 R1KK=RTURB                                                        NOXX    181
      R1K=0.0                                                           NOXX    182
      R1I=0.0                                                           NOXX    183
      GO TO 299                                                         NOXX    184
  297 R1K=RTURB                                                         NOXX    185
      R1KK=0.0                                                          NOXX    186
      R1I=0.0                                                           NOXX    187
      GO TO 299                                                         NOXX    188
  296 R1I=RTURB                                                         NOXX    189
      R1K=0.0                                                           NOXX    190
      R1KK=0.0                                                          NOXX    191
      GO TO 299                                                         NOXX    192
  294 R1I=RLAM                                                          NOXX    193
      R1K=RLAM                                                          NOXX    194
      R1KK=RLAM                                                         NOXX    195
      R1=RLAM                                                           NOXX    196
      EN=3.0D0                                                          NOXX    197
  299 CONTINUE                                                          NOXX    198
  290 RN=R1*EN                                                          CALC    202
      IF(.NOT.LNRG)GO TO 205                                            NOXX    199
      IF(RTURB.LT.RLAM)GO TO 205                                        NOXX    200
      RT=R1*(TEN(J)+TK1-EN)                                             NOXX    201
      GO TO 205                                                         CALC    204
C                                                                       CALC    205
  201 R1=R1*RHSM*RHOP*S2(I)                                             CALC    206
      RLAM=R1                                                           NOXX    202
      PHI=S2(I)                                                         NOXX    203
      RTURB=CEBU(J)*RHOP*PHI*EDKIJ                                      NOXX    204
      R1I=DMIN1(RLAM,RTURB)                                             NOXX    205
      R1=R1I                                                            NOXX    206
      RN=R1                                                             CALC    207
      IF(.NOT.LNRG)GO TO 205                                            NOXX    207
      IF(RTURB.LT.RLAM)GO TO 205                                        NOXX    208
      RT=R1*(TEN(J)+TK1-2.0D0)                                          NOXX    209
      GO TO 205                                                         CALC    209
C                                                                       CALC    210
  202 R1=R1*RHSM*S2(I)*RHSQ*S2(K)                                       CALC    211
      RLAM=R1                                                           NOXX    210
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      PHI=DMIN1(S2(K),S2(I))                                            NOXX    211
      RTURB=CERU(J)*PHOP*PHI*EDKIJ                                      NOXX    212
      IF(RLAP.LT.RTURB)GO TO 301                                        NOXX    213
      R1=RTURB                                                          NOXX    214
      EN=1.000                                                          NOXX    215
      IF(S2(K).LT.S2(I))GO TO 302                                       NOXX    216
      R1I=RTURB                                                         NOXX    217
      R1K=0.0                                                           NOXX    218
      GO TO 303                                                         NOXX    219
  302 R1I=0.0                                                           NOXX    220
      R1K=RTURB                                                         NOXX    221
      GO TO 303                                                         NOXX    222
  301 R1I=RLAM                                                          NOXX    223
      R1K=RLAM                                                          NOXX    224
      R1=RLAM                                                           NOXX    225
      EN=2.000                                                          NOXX    226
  303 CONTINUE                                                          NOXX    227
      RN=R1*EN                                                          NOXX    228
      IF(.NOT.LNR6)GO TO 205                                            NOXX    229
      IF(RTURB.LT.RLAM)GO TO 205                                        NOXX    230
      RT=R1*(TEN(J)+TK1-3.000)                                          NOXX    231
C                                                                       CALC    214
  205 TM1=R1                                                            CALC    215
C                                                                       CALC    216
C                                                                       CALC    217
C-----CALCULATE REVERSE RATE CONST FROM FWD RATE CONST AND EQUIL CONST  CALC    218
C-----WHENEVER TEMP IS LESS THAN 1500 K                                 CALC    219
C                                                                       CALC    220
      IF (TK.GT.1500.000) GO TO 220                                     CALC    221
C                                                                       CALC    222
      HH=HO(I)-HO(M)                                                    CALC    223
      SS=SO(I)-SO(M)                                                    CALC    224
      IF (NODF-2) 210,211,212                                           CALC    225
C                                                                       CALC    226
  210 HH=HH+HO(K)-HO(N)                                                 CALC    227
      SS=SS+SO(K)-SO(N)                                                 CALC    228
      IF(KK.EQ.0) GO TO 218                                             CALC    229
      HH=HH+HO(KK)                                                      CALC    230
      SS=SS+SO(KK)                                                      CALC    231
  218 IF(NN.EQ.0) GO TO 219                                             CALC    232
      HH=HH-HO(NN)                                                      CALC    233
      SS=SS-SO(NN)                                                      CALC    234
  219 CONTINUE                                                          CALC    235
      RXX=RX(J)+SS                                                      CALC    236
      TK2=TK1+HH                                                        CALC    237
      TN2=TEN(J)                                                        CALC    238
      GO TO 230                                                         CALC    239
C                                                                       CALC    240
  211 HH=HH-HO(N)                                                       CALC    241
      SS=SS-SO(N)                                                       CALC    242
C     -2.500304 IS E-LOG OF GAS CONST 0.08206 M**3-ATM/KGMOL-DEG K.     CALC    243
      RXX=RX(J)+SS-2.50030400                                           CALC    244
      TK2=TK1+HH                                                        CALC    245
      TN2=TEN(J)+1.000                                                  CALC    246
      GO TO 230                                                         CALC    247
C                                                                       CALC    248
  212 HH=HH+HO(K)                                                       CALC    249
      SS=SS+SO(K)                                                       CALC    250
      RXX=RX(J)+SS+2.50030400                                           CALC    251
      TK2=TK1+HH                                                        CALC    252
      TN2=TEN(J)-1.000                                                  CALC    253
      GO TO 230                                                         CALC    254
C                                                                       CALC    255
  220 RXX=RX2(J)                                                        CALC    256
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      TM2=TACT2(J)*TKINV                                          CALC    257
      TN2=TEN2(J)                                                 CALC    258
C                                                                 CALC    259
  230 TM2=TK2-BXX                                                 CALC    260
      IF (TN2.NE.0.D0) TM2=TM2-TN2*TLN                            CALC    261
      IF (DABS(TM2).GT.BIG) GO TO 250                             CALC    262
      R2=DEXP(-TM2)                                               CALC    263
C-----MULTIPLY HOMOGENEOUS RATE CONSTANT BY CONTACT INDEX         CALC    264
      R2=R2*X2(J)                                                 CALC    265
C                                                                 CALC    266
      IF (MODE-2) 240,241,242                                     CALC    267
C                                                                 CALC    268
  240 R2=R2*S2(M)*RHSQ*S2(N)                                      CALC    269
      RLAM=R2                                                     NOXX    232
      PHI=DMIN1(S2(M),S2(N))                                      NOXX    233
      RTURB=CERU(J)*RHOP*PHI*EDKIJ                                NOXX    234
      IF(RLAM.LT.RTURB)GO TO 311                                  NOXX    235
      R2=RTURB                                                    NOXX    236
      EN=1.000                                                    NOXX    237
      IF(S2(M).LT.S2(N))GO TO 312                                 NOXX    238
      R2N=RTURB                                                   NOXX    239
      R2M=0.0                                                     NOXX    240
      GO TO 313                                                   NOXX    241
  312 R2N=0.0                                                     NOXX    242
      R2M=RTURB                                                   NOXX    243
      GO TO 313                                                   NOXX    244
  311 R2N=RLAM                                                    NOXX    245
      R2M=RLAM                                                    NOXX    246
      R2=RLAM                                                     NOXX    247
      EN=2.000                                                    CALC    270
  313 CONTINUE                                                    NOXX    248
      IF(NN.EQ.0) GO TO 249                                       CALC    271
      RLAM=RLAM*RHOP*S2(NN)                                       NOXX    249
      PHI=DMIN1(PHI,S2(NN))                                       NOXX    250
      RTURB=CERU(J)*RHOP*PHI*EDKIJ                                NOXX    251
      IF(RLAM.LT.RTURB)GO TO 314                                  NOXX    252
      R2=RTURB                                                    NOXX    253
      EN=1.000                                                    NOXX    254
      IF(S2(M).LT.S2(N))GO TO 315                                 NOXX    255
      IF(S2(N).LT.S2(NN))GO TO 316                                NOXX    256
      GO TO 318                                                   NOXX    257
  315 IF(S2(M).LT.S2(NN))GO TO 317                                NOXX    258
  318 R2NN=RTURB                                                  NOXX    259
      R2M=0.0                                                     NOXX    260
      R2N=0.0                                                     NOXX    261
      GO TO 319                                                   NOXX    262
  317 R2M=RTURB                                                   NOXX    263
      R2NN=0.0                                                    NOXX    264
      R2N=0.0                                                     NOXX    265
      GO TO 319                                                   NOXX    266
  316 R2N=RTURB                                                   NOXX    267
      R2NN=0.0                                                    NOXX    268
      R2M=0.0                                                     NOXX    269
      GO TO 319                                                   NOXX    270
  314 R2N=RLAM                                                    NOXX    271
      R2M=RLAM                                                    NOXX    272
      R2NN=RLAM                                                   NOXX    273
      R2=RLAM                                                     NOXX    274
      EN=3.000                                                    NOXX    275
  319 CONTINUE                                                    NOXX    276
  249 RN=RN-R2*EN                                                 CALC    274
      IF(.NOT.LNRG)GO TO 250                                      NOXX    277
      IF(RTURB.LT.RLAM)GO TO 250                                  NOXX    278
      RT=RT-R2*(TN2+TM2-EN)                                       NOXX    279
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      GO TO 250                                                          CALC    276
C                                                                        CALC    277
  241 R2=R2*RHSM*S2(M)*RHSQ*S2(N)                                        CALC    278
      RLAM=R2                                                            NOXX    280
      PHI=DMIN1(S2(M),S2(N))                                             NOXX    281
      RTURB=CEBU(J)*RHOP*PHI*EDKIJ                                       NOXX    282
      IF(RLAM.LT.RTURB)GO TO 321                                         NOXX    283
      R2=RTURB                                                           NOXX    284
      FN=1.000                                                           NOXX    285
      IF(S2(M).LT.S2(N))GO TO 322                                        NOXX    286
      R2M=RTURB                                                          NOXX    287
      R2N=0.0                                                            NOXX    288
      GO TO 323                                                          NOXX    289
  322 R2N=0.0                                                            NOXX    290
      R2M=RTURB                                                          NOXX    291
      GO TO 323                                                          NOXX    292
  321 R2M=RLAM                                                           NOXX    293
      R2N=RLAM                                                           NOXX    294
      R2=RLAM                                                            NOXX    295
      FN=2.000                                                           NOXX    296
  323 CONTINUE                                                           NOXX    297
      RN=RN-R2*FN                                                        NOXX    298
      IF(.NOT.LNRG)GO TO 250                                             NOXX    299
      IF(RTURB.LT.RLAM)GO TO 250                                         NOXX    300
      RT=RT-R2*(TN2+TK2-3.000)                                           NOXX    301
      GO TO 250                                                          CALC    281
C                                                                        CALC    282
  242 R2=R2*RHSM*RHOP*S2(M)                                              CALC    283
      RLAM=R2                                                            NOXX    302
      PHI=S2(M)                                                          NOXX    303
      RTURB=CEBU(J)*RHOP*PHI*EDKIJ                                       NOXX    304
      R2M=DMIN1(RLAM,RTURB)                                              NOXX    305
      R2=R2M                                                             NOXX    306
      RN=RN-R2                                                           CALC    284
      IF(.NOT.LNRG)GO TO 250                                             NOXX    307
      IF(RTURB.LT.RLAM)GO TO 250                                         NOXX    308
      RT=RT-R2*(TN2+TK2-2.000)                                           NOXX    309
C                                                                        CALC    286
  250 TM1=TM1-R2                                                         CALC    287
C                                                                        CALC    288
C                                                                        CALC    289
C  ***KINETIC***                                                         CALC    290
C  DERIVATIVE AND FUNCTION MATRIX FOR KINETIC SOLUTION                   CALC    291
C                                                                        CALC    292
      A(I,I)=A(I,I)+R1I                                                  NOXX    310
      A(M,I)=A(M,I)-R1I                                                  NOXX    311
      A(I,M)=A(I,M)-R2M                                                  NOXX    312
      A(M,M)=A(M,M)+R2M                                                  NOXX    313
      A(I,NSM)=A(I,NSM)-RN                                               CALC    297
      A(M,NSM)=A(M,NSM)+RN                                               CALC    298
      A(I,NQ)=A(I,NQ)+RT                                                 CALC    299
      A(M,NQ)=A(M,NQ)-RT                                                 CALC    300
      A(I,NA)=A(I,NA)-TM1                                                CALC    301
      A(M,NA)=A(M,NA)+TM1                                                CALC    302
      IF (MODE.EQ.3) GO TO 260                                           CALC    303
C                                                                        CALC    304
      A(N,I)=A(N,I)-R1I                                                  NOXX    314
      A(N,M)=A(N,M)+R2M                                                  NOXX    315
      A(I,N)=A(I,N)-R2N                                                  NOXX    316
      A(M,N)=A(M,N)+R2N                                                  NOXX    317
      A(N,N)=A(N,N)+R2N                                                  NOXX    318
      A(N,NSM)=A(N,NSM)+RN                                               CALC    310
      A(N,NQ)=A(N,NQ)-RT                                                 CALC    311
      A(N,NA)=A(N,NA)+TM1                                                CALC    312
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      IF (MODE.EQ.2) GO TO 270                                          CALC  313
C                                                                       CALC  314
  260 CONTINUE                                                          CALC  315
      A(K,I)=A(K,1)*R1I                                                 NOXX  319
      A(I,K)=A(I,K)*R1K                                                 NOXX  320
      A(K,K)=A(K,K)*R1K                                                 NOXX  321
      A(M,K)=A(M,K)-R1K                                                 NOXX  322
      A(K,M)=A(K,M)-R2M                                                 NOXX  323
      A(K,NSM)=A(K,NSM)-RN                                              CALC  321
      A(K,NQ)=A(K,NQ)*RT                                                CALC  322
      A(K,NA)=A(K,NA)-TM1                                               CALC  323
      IF (MODE.EQ.3) GO TO 270                                          CALC  324
C                                                                       CALC  325
      A(N,K)=A(N,K)-R1K                                                 NOXX  324
      A(K,N)=A(K,N)-R2N                                                 NOXX  325
      IF(KK.EQ.0) GO TO 268                                             CALC  326
      A(I,KK)=A(I,KK)+R1KK                                              NOXY  326
      A(K,KK)=A(K,KK)+R1KK                                              NOXX  327
      A(KK,I)=A(KK,I)+R1I                                               NOXX  328
      A(KK,K)=A(KK,K)+R1K                                               NOXX  329
      A(KK,KK)=A(KK,KK)+R1KK                                            NOXX  330
      A(M,KK)=A(M,KK)-R1KK                                              NOXX  331
      A(N,KK)=A(N,KK)-R1KK                                              NOXX  332
      A(KK,M)=A(KK,M)-R2M                                               NOXX  333
      A(KK,N)=A(KK,N)-R2N                                               NOXX  334
      A(KK,NSM)=A(KK,NSM)-RN                                            CALC  338
      A(KK,NQ)=A(KK,NQ)+RT                                              CALC  339
      A(KK,NA)=A(KK,NA)-TM1                                             CALC  340
  268 IF(NN.EQ.0) GO TO 269                                             CALC  341
      A(I,NN)=A(I,NN)-R2NN                                              NOXX  335
      A(K,NN)=A(K,NN)-R2NN                                              NOXX  336
      A(NN,I)=A(NN,I)-R1I                                               NOXX  337
      A(NN,K)=A(NN,K)-R1K                                               NOXX  338
      A(M,NN)=A(M,NN)+R2NN                                              NOXX  339
      A(N,NN)=A(N,NN)+R2NN                                              NOXX  340
      A(NN,M)=A(NN,M)+R2M                                               NOXX  341
      A(NN,N)=A(NN,N)+R2N                                               NOXX  342
      A(NN,NN)=A(NN,NN)+R2NN                                            NOXX  343
      A(NN,NSM)=A(NN,NSM)+RN                                            CALC  351
      A(NN,NQ)=A(NN,NQ)-RT                                              CALC  352
      A(NN,NA)=A(NN,NA)+TM1                                             CALC  353
  269 CONTINUE                                                          CALC  354
C                                                                       CALC  355
  270 CONTINUE                                                          CALC  356
C                                                                       CALC  357
  271 CONTINUE                                                          &STEP  603
      HSUM=0.000                                                        CALC  358
      DO 280 I=1,NS                                                     CALC  359
      S2I=S2(I)                                                         CALC  360
      A(I,I)=A(I,I)+ENV*S2I                                             CALC  361
      A(I,NA)=A(I,NA)+ENV*(S1(I)-S2I)                                   CALC  362
      A(NSM,I)=S2I                                                      CALC  363
      A(NSM,NA)=A(NSM,NA)-S2I                                           CALC  364
      A(NQ,I)=HQ(I)*S2I                                                 CALC  365
      HSUM=HSUM+A(NQ,I)                                                 CALC  366
  280 CONTINUE                                                          CALC  367
C                                                                       CALC  368
      A(NSM,NSM)=-SM                                                    CALC  369
C-----A(NSM,NQ) AND A(NQ,NSM) ARE EQUAL TO ZERO.                        CALC  370
      A(NSM,NA)=A(NSM,NA)+SM                                            CALC  371
      A(NQ,NQ)=CPSUM+QDRV                                               CALC  372
      A(NQ,NA)=HIN-Q-HSUM                                               CALC  373
      IMAT=NQ                                                           CALC  374
      IF(LENER)GO TO 282                                                NOXX  344
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      IMAT=NS                                                          NOXX    345
      DO 281 I=1,NS                                                    NOXX    346
  281 A(I,NSM1)=A(I,NA)                                                NOXX    347
  282 CONTINUE                                                         NOXX    348
      GO TO 400                                                        CALC    375
C                                                                      CALC    376
C***   ***   ***   ***   ***   ***   ***   ***   CHAPTER 3   ***   ***  CALC    377
C***   ***   ***   ***   ***   ***   ***   ***   CHAPTER 3   ***   ***  CALC    378
C                                                                      CALC    379
C  ***EQUILIBRIUM***                                                   CALC    380
C  DERIVATIVE AND FUNCTION MATRIX FOR EQUILIBRIUM SOLUTION             CALC    381
C                                                                      CALC    382
  300 DO 310 L=1,NLM                                                   CALC    383
  310 RO(L)=0.0D0                                                      CALC    384
C                                                                      CALC    385
      HSUM=0.0D0                                                       CALC    386
      SUM=0.0D0                                                        CALC    387
      DO 340 I=1,NS                                                    CALC    388
      SUM=SUM+S2(I)                                                    CALC    389
      TM1=HO(I)*S2(I)                                                  CALC    390
      HSUM=HSUM+TM1                                                    CALC    391
      TM2=(HO(I)-SO(I)+Y(I)-Y(NSM)+PPLN)*S2(I)                         CALC    392
      A(N1,N3)=A(N1,N3)+TM2                                            CALC    393
      A(N2,N2)=A(N2,N2)+HO(I)*TM1                                      CALC    394
      A(N2,N3)=A(N2,N3)+HO(I)*TM2                                      CALC    395
C                                                                      CALC    396
      DO 330 L=1,NLM                                                   CALC    397
      IF (AL(L,I).EQ.0.0D0) GO TO 330                                  CALC    398
      TM3=AL(L,I)*S2(I)                                                CALC    399
C-----CROSS-DERIVATIVES OF ELEMENT EQUATIONS, D F(L)/D PI(K)            CALC    400
      DO 320 K=L,NLM                                                   CALC    401
      IF (AL(K,I).EQ.0.0D0) GO TO 320                                  CALC    402
      A(L,K)=A(L,K)+AL(K,I)*TM3                                        CALC    403
  320 CONTINUE                                                         CALC    404
C-----DERIVATIVES OF L-ELEMENT EQN W.R.T. LN SM AND LN T                CALC    405
      A(L,N1)=A(L,N1)+TM3                                              CALC    406
      A(L,N2)=A(L,N2)+AL(L,I)*TM1                                      CALC    407
C-----NEGATIVE OF L-ELEMENT EQN, F(L)                                  CALC    408
      A(L,N3)=A(L,N3)+AL(L,I)*TM2                                      CALC    409
      RO(L)=RO(L)+AL(L,I)*S1(I)                                        CALC    410
  330 CONTINUE                                                         CALC    411
  340 CONTINUE                                                         CALC    412
C                                                                      CALC    413
      A(N1,N1)=SUM-SM                                                  CALC    414
      A(N1,N3)=A(N1,N3)-(SUM-SM)                                       CALC    415
      A(N1,N2)=HSUM                                                    CALC    416
      A(N2,N2)=A(N2,N2)+CPSUM+ODRV                                     CALC    417
      A(N2,N3)=A(N2,N3)+HIN-HSUM-O                                     CALC    418
C                                                                      CALC    419
C-----NEGATIVE OF L-ELEMENT EQNS, F(L)                                 CALC    420
      DO 350 L=1,NLM                                                   CALC    421
      A(L,N3)=A(L,N3)+RO(L)-A(L,N1)                                    CALC    422
  350 CONTINUE                                                         CALC    423
C                                                                      CALC    424
C-----STORE SYMPETRIC ELEMENTS OF MATRIX                               CALC    425
C                                                                      CALC    426
      DO 360 I=1,N2                                                    CALC    427
      DO 360 J=I,N2                                                    CALC    428
      A(J,I)=A(I,J)                                                    CALC    429
  360 CONTINUE                                                         CALC    430
C                                                                      CALC    431
C-----INTERCHANGE SM-EQN WITH ELEMENT ROW L WITH LARGEST A(L,N1) TO     CALC    432
C-----AVOID POTENTIAL ZERO IN DIAGONAL ELEMENT A(N1,N1)                 CALC    433
C                                                                      CALC    434
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      TM1=0.000                                                          CALC  435
      DO 370 L=1,NLM                                                     CALC  436
      IF (A(L,N1).LT.TM1) GO TO 370                                      CALC  437
      TM1=A(L,N1)                                                        CALC  438
      LL=L                                                               CALC  439
  370 CONTINUE                                                           CALC  440
C                                                                        CALC  441
      DO 380 J=1,N3                                                      CALC  442
      TM1=A(N1,J)                                                        CALC  443
      A(N1,J)=A(LL,J)                                                    CALC  444
      A(LL,J)=TM1                                                        CALC  445
  380 CONTINUE                                                           CALC  446
      IMAT=N2                                                            CALC  447
C                                                                        CALC  448
C****    ****    ****    ****    ****    ****    CHAPTER 4   ****  ***  CALC  449
C****    ****    ****    ****    ****    ****    CHAPTER 4   ****  ***  CALC  450
C                                                                        CALC  451
C  ***MATRIX SOLUTION***                                                 CALC  452
C  SOLVE FOR CORRECTIONS BY STANDARD PIVOTAL GAUSSIAN ELIMINATION        CALC  453
C                                                                        CALC  454
  400 KMAT=IMAT+1                                                        CALC  455
C-----OPTIONAL OUTPUT OF INTERMEDIATE VALUES FOR DEBUGGING               CALC  456
      IF (.NOT.LDEBUG) GO TO 410                                         CALC  457
      IF (NDEBUG.LT.5) GO TO 410                                         CALC  458
      WRITE(6,401)                                                       CALC  459
  401 FORMAT(1H0,10X,36HELEMENTS A(I,K) OF CORRECTION MATRIX/)           CALC  460
      DO 403 K=1,IMAT                                                    CALC  461
      WRITE(6,402) (A(K,I),I=1,KMAT)                                     CALC  462
  402 FORMAT(1X,1P16D8.0)                                                CALC  463
  403 CONTINUE                                                           CALC  464
  410 CONTINUE                                                           CALC  465
      DO 450 NN=1,IMAT                                                   CALC  466
      IF (A(NN,NN).EQ.0.0D0) GO TO 900                                   CALC  467
C-----CHANGE 1.0D0 TO 1.0 FOR NON-IBM MACHINES NOT REQUIRING DOUBLE PRE  CALC  468
C     DTM1=1.0D0/A(NN,NN)                                                CALC  469
      DTM1=1.0D0/A(NN,NN)                                                CALC  470
      K=NN+1                                                             CALC  471
      DO 420 J=K,KMAT                                                    CALC  472
      A(NN,J)=A(NN,J)*DTM1                                               CALC  473
  420 CONTINUE                                                           CALC  474
      IF (K.EQ.KMAT) GO TO 450                                           CALC  475
      DO 440 I=K,IMAT                                                    CALC  476
      IF (A(I,NN).EQ.0.000) GO TO 440                                    CALC  477
      DO 430 J=K,KMAT                                                    CALC  478
      A(I,J)=A(I,J)-A(I,NN)*A(NN,J)                                      CALC  479
  430 CONTINUE                                                           CALC  480
  440 CONTINUE                                                           CALC  481
  450 CONTINUE                                                           CALC  482
C                                                                        CALC  483
C-----BACK SOLVE FOR CORRECTION VECTOR                                   CALC  484
C                                                                        CALC  485
      K=IMAT                                                             CALC  486
  460 J=K+1                                                              CALC  487
      DSUM=0.000                                                         CALC  488
      X(K)=0.000                                                         CALC  489
      IF (IMAT.LT.J) GO TO 480                                           CALC  490
      DO 470 I=J,IMAT                                                    CALC  491
      DSUM=DSUM+A(K,I)*X(I)                                              CALC  492
  470 CONTINUE                                                           CALC  493
  480 CONTINUE                                                           CALC  494
      X(K)=A(K,KMAT)-DSUM                                                CALC  495
      K=K-1                                                              CALC  496
      IF (K.NE.0) GO TO 460                                              CALC  497
C                                                                        CALC  498
```

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      RETURN                                                                    CALC      499
C                                                                               CALC      500
C*****     *****     *****     *****     *****  CHAPTER 5  *****  *           CALC      501
C*****     *****     *****     *****     *****  CHAPTER 5  *****  *           CALC      502
C                                                                               CALC      503
C  ***SINGULAR MATRIX***                                                        CALC      504
C                                                                               CALC      505
  500 WRITE(6,501)                                                              CALC      506
  501 FORMAT(1HO,10X,3(4H****),16HSINGULAR MATRIX/)                             CALC      507
C-----SET LCONVG=.TRUE. TO NOTIFY SPECE OF SINGULAR MATRIX                      CALC      508
      LCONVG=.TRUE.                                                             CALC      509
      RETURN                                                                    CALC      510
       END                                                                      CALC      511
      SUBROUTINE SPECE                                                          SPEC        2
C                                                                               SPEC        3
      DOUBLE PRECISION AL,BO,CPSUN,ENV,ER,FO,HSUBO,HSUM,HO,PA,PI,PPLN,          NOXX      349
     1 QO,Q1,Q2,Q3,Q4,RGAS,RGASIN,RHOP,SM,SMINV,SMW,SSAVE,SO,S1,S2,TK,          NOXXX      17
     2 TKINV,TLN,Z,SMO                                                          NOXXX      18
      DOUBLE PRECISION X,Y                                                      NOXXX      19
      DOUBLE PRECISION ETA,ETAO,ETA1,SUM,TINY,TM1,TNY,TST1,VM,VP                NOXX      350
      LOGICAL LADIAB,LCONVG,LDEBUG,LEQUIL,LNRG,LREACT,LENER                     NOXX      351
C                                                                               SPEC        6
      COMMON                                                                    SPEC        7
     3/CCHEMI/CPSUP,HSUM,FO,PPLN,RGAS,RGASIN,SMINV,TKINV,TLN,LNRG               NOXX      352
     1/CEQUIL/AL(7,30),ATOM(3,7),BO(7),PI(7)                                    SPEC        9
     1/CINDEX/IDCO,IDFU,IDO2,IDN2,IDH2O,IDCO2,IDH1,IDH2,IDN1,IDNO,IDNO2         NOXX      353
     1,IDO,IDOH,IHCPS,ILC,ILH,IMAT,ITER,JJ,N1,N2,N3,NA,NGLOB,NGLORP,            NOXX      354
     2 NLM,NO,NSM,NS1,NS2,IDCH                                                  4STEP     604
     1/CMATRI/X(32),Y(32)                                                       NOXX      356
     1/CPARAM/ASUB(30,3),ENV,ER,HSUBO,NDEBUG,NS,PA,QO,Q1,Q2,Q3,Q4,RHOP,         SPEC       13
     1 SM,SMW(30),SMO,S1(30),S2(30),TK,LADIAB,LDEBUG,LEQUIL,LREACT,LENER        NOXX      357
     2,FDKIJ,LCONVG                                                             NOXX      358
     1/CSPECE/HO(30),SO(30),SSAVE(30),Z(7,2,30)                                 NOXX      359
C                                                                               SPEC       16
C*******************************************************************************SPEC       17
C     THIS SUBROUTINE CALLS CALC TO COMPUTE THE CORRECTIONS TO THE              SPEC       18
C     CHEMICAL SPECIES AND TEMP AND DETERMINES THE UNDERRELAXATION              SPEC       19
C     PARAMETER PRIOR TO THE APPLICATION OF THESE CORRECTIONS TO THE            SPEC       20
C     ESTIMATES FOR BOTH EQUILIBRIUM AND KINETIC STATIONARY STATES              SPEC       21
C     FOR EACH ITERATION.  SPECE ALSO CONTROLS THE CONVERGENCE TESTS            SPEC       22
C     REFERENCE  CREK    (WASHINGTON STATE UNIVERSITY)  MARCH 1976              SPEC       23
C*******************************************************************************SPEC       24
C                                                                               SPEC       25
      DATA ITMAX/50/,TINY/1.0D-20/,TNY/-46.051700/                              NOXX      360
C                                                                               SPEC       27
      LCONVG=.FALSE.                                                            SPEC       28
      SM=0.000                                                                  NOXX      361
      DO 20 I=1,NS                                                              SPEC       30
      IF (S2(I).GT.TINY) GO TO 10                                               SPEC       31
      S2(I)=TINY                                                                SPEC       32
      Y(I)=TNY                                                                  SPEC       33
      GO TO 20                                                                  SPEC       34
   10 SM=SM+S2(I)                                                               SPEC       35
      Y(I)=DLOG(S2(I))                                                          SPEC       36
   20 CONTINUE                                                                  SPEC       37
      TKINV=1.000/TK                                                            SPEC       38
      TLN=DLOG(TK)                                                              SPEC       39
      Y(NSM)=DLOG(SM)                                                           SPEC       40
      SMINV=1.000/SM                                                            SPEC       41
      Y(NO)=TLN                                                                 SPEC       42
C                                                                               SPEC       43
C* * * * * * * * * * * * * * * * * * * * * * CHAPTER 1 * * * * * * *           SPEC       44
C* * * * * * * * * * * * * * * * * * * * * * CHAPTER 1 * * * * * * *           SPEC       45
C                                                                               SPEC       46
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C  ***SOLVE FOR CORRECTIONS***                                                  SPEC     47
C  INITIATE THE ITER LOOP AND CALL CALC TO SET UP AND CALCULATE THE            SPEC     48
C  CORRECTIONS FOR EITHER EQUILIBRIUM OR KINETIC SOLUTION                      SPEC     49
C                                                                              SPEC     50
      ETA=1.000                                                                SPEC     51
      ETAO=ETA                                                                 SPEC     52
      NDEC=0                                                                   SPEC     53
      NRLX=0                                                                   SPEC     54
      DO 350 ITER=1,ITMAX                                                      SPEC     55
C                                                                              SPEC     56
      CALL CALC                                                                SPEC     57
C                                                                              SPEC     58
      IF (IMAT.EQ.NQ) GO TO 300                                                SPEC     59
      IF(IMAT.EQ.NS)GO TO 300                                                  NOXX    362
C                                                                              SPEC     60
C                                                                              SPEC     61
C**  **  **  **  **  **  **  **  **  **  **  **  CHAPTER 2  **  **  **         SPEC     62
C**  **  **  **  **  **  **  **  **  **  **  **  CHAPTER 2  **  **  **         SPEC     63
C                                                                              SPEC     64
C  ***CONSTRUCT CORRECTIONS FOR EQUILIBRIUM SPECIES***                         SPEC     65
C  CHECK FOR SINGULAR MATRIX (LCONVG SET TO TRUE AT END OF CALC)               SPEC     66
      IF (.NOT.LCONVG) GO TO 200                                               SPEC     67
      LCONVG=.FALSE.                                                           SPEC     68
      RETURN                                                                   SPEC     69
C                                                                              SPEC     70
  200 DO 210 L=1,NLM                                                           SPEC     71
  210 PI(L)=X(L)                                                               SPEC     72
      X(NSM)=X(N1)                                                             SPEC     73
      X(NQ)=X(N2)                                                              SPEC     74
      DO 230 I=1,NS                                                            SPEC     75
      X(I)=HO(I)*X(NQ)-(HO(I)-SO(I)+Y(I)+PPLN-Y(NSM))+X(NSM)                   SPEC     76
      DO 220 L=1,NLM                                                           SPEC     77
      X(I)=X(I)+AL(L,I)*PI(L)                                                  SPEC     78
  220 CONTINUE                                                                 SPEC     79
  230 CONTINUE                                                                 SPEC     80
C                                                                              SPEC     81
C***   ***   ***   ***   ***   ***   ***   ***   CHAPTER 3   ***   ***       SPEC     82
C***   ***   ***   ***   ***   ***   ***   ***   CHAPTER 3   ***   ***       SPEC     83
C                                                                              SPEC     84
C  ***CALCULATE UNDERRELAXATION PARAMETER ETA***                               SPEC     85
C  UNDERRELAXATION TESTS ARE DIFFERENT FOR MAJOR AND MINOR SPECIES WITH        SPEC     86
C  ETA = MIN(ETA1,ETA2,1)  WHERE                                               SPEC     87
C  MAJOR SPECIES ---  S2(I)/SM   1.0D-8                                        SPEC     88
C  MINOR SPECIES ---  S2(I)/SM   1.0D-8                                        SPEC     89
C  AND ONLY POSITIVE CORRECTION CHANGES FOR MOLE NUMBERS ARE MONITORED         SPEC     90
C  ETA1 = MAJOR SPECIES CONTROL                                                SPEC     91
C  ETA2 = MINOR SPECIES CONTROL                                                SPEC     92
C                                                                              SPEC     93
  300 ETAO=ETA                                                                 SPEC     94
      ETA=1.000                                                                SPEC     95
      ETA1=1.000                                                               SPEC     96
      SUM=DABS(X(NSP))                                                         SPEC     97
      TM1=DABS(X(NQ))                                                          SPEC     98
      IF (TM1.GT.SUM) SUM=TM1                                                  SPEC     99
      DO 320 I=1,NS                                                            SPEC    100
      IF (X(I).LE.0.000) GO TO 320                                             SPEC    101
      IF (S2(I)*SMINV.LE.1.0D-8) GO TO 310                                     SPEC    102
C-----MAJOR SPECIES                                                            SPEC    103
      IF (X(I).GT.SUM) SUM=X(I)                                                SPEC    104
      GO TO 320                                                                SPEC    105
C-----MINOR SPECIES                                                            SPEC    106
  310 TST1=DABS((Y(NSM)-Y(I)-11.512925D0)/((X(I)-X(NSM))+TINY))                NOXX    363
      IF (TST1.LT.ETA1) ETA1=TST1                                              SPEC    108
  320 CONTINUE                                                                 SPEC    109
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      IF(SUM.GT.0.200)ETA=0.200/SUM                                    NOXX      364
      IF (ETA1.LT.ETA) ETA=ETA1                                        SPEC      111
      IF(LEQUIL)GO TO 400                                              SPEC      112
C                                                                      SPEC      113
C   ***CONVERGENCE MONITORING***                                       SPEC      114
C   AFTER TEN SUCCESSIVE UNDERRELAXED ITERATIONS, IN WHICH ETA DOES NOT SPEC      115
C   INCREASE BY 1.1 OR MORE, OR AFTER SIX ITERATIONS IN WHICH ETA      NOXX      365
C   DECREASES, DIVERGENCE IS ASSUMED AND THE SOLUTION TERMINATED       SPEC      117
C                                                                      SPEC      118
C   LNRG=.TRUE. ----  FULL EQUATIONS                                   SPEC      119
      IF (ETA.EQ.1.0D0) NRLX=-1                                        SPEC      120
      IF((ETA/ETA0).GE.1.1D0)NRLX= 1                                   NOXX      366
      NRLX=NRLX+1                                                      SPEC      122
      IF (NRLX.GT.10) GO TO 900                                        SPEC      123
      IF (ETA.LT.ETA0) NDEC=NDEC+1                                     SPEC      124
      IF (.NOT.LNRG) NDEC=1                                            SPEC      125
      IF (NDEC.GT.6) GO TO 900                                         SPEC      126
C                                                                      SPEC      127
C****    ****    ****    ****    ****    ****    CHAPTER 4   ****  ***  SPEC      128
C****    ****    ****    ****    ****    ****    CHAPTER 4   ****  ***  SPEC      129
C                                                                      SPEC      130
C   APPLY CORRECTIONS TO ESTIMATES                                     SPEC      131
C                                                                      SPEC      132
C                                                                      SPEC      133
  400 CONTINUE                                                         SPEC      134
      SUM=0.0D0                                                        NOXX      367
      DO 420 I=1,NS                                                    SPEC      135
      Y(I)=Y(I)+ETA*X(I)                                               SPEC      136
      IF (Y(I).LT.TNY) GO TO 410                                       SPEC      137
      S2(I)=DEXP(Y(I))                                                 SPEC      138
      SUM=SUM+S2(I)*SMW(I)                                             NOXX      368
      GO TO 420                                                        SPEC      139
C                                                                      SPEC      140
  410 Y(I)=TNY                                                         SPEC      141
      S2(I)=TINY                                                       SPEC      142
C-----INSURE CONVERGENCE TEST PASSED WHENEVER Y(I)=TNY                 SPEC      143
      X(I)=0.0D0                                                       SPEC      144
  420 CONTINUE                                                         SPEC      145
      DO 450 I=1,NS                                                    NOXX      369
      S2(I)=S2(I)/SUM                                                  NOXX      370
  450 Y(I)=DLOG(S2(I))                                                 NOXX      371
      Y(NSM)=Y(NSM)+ETA*X(NSM)                                         SPEC      146
      SM=DEXP(Y(NSM))                                                  SPEC      147
      SMINV=1.0D0/SM                                                   SPEC      148
      Y(NQ)=Y(NQ)+ETA*X(NQ)                                            SPEC      149
      TLN=Y(NQ)                                                        SPEC      150
      TK=DEXP(TLN)                                                     SPEC      151
      TKINV=1.0D0/TK                                                   SPEC      152
C                                                                      SPEC      153
      IF (.NOT.LDEBUG) GO TO 500                                       SPEC      154
      IF (NDEBUG.GE.3) WRITE(6,430) ITER,ETA,LREACT,LEQUIL,LADIAB,     SPEC      155
     1                              LNRG,HSUBQ,SM,EMV,TK               SPEC      156
      IF (NDEBUG.GE.4) WRITE(6,440) (I,ASUB(I,1),S1(I),S2(I),Y(I),     SPEC      157
     1                               X(I),HO(I),SO(I),I=1,NS)          SPEC      158
  430 FORMAT(2X,I3,1PD12.3,4L8,1P4D12.3)                               SPEC      159
  440 FORMAT(20X,7HSPECIES,4X,5HS1(I),7X,5HS2(I),7X,4HY(I),8X,         SPEC      160
     A4HX(I),8X,5HHO(I),7X,5HSO(I)/(16X,I2,3X,A4,2X,1P6D12.3))         SPEC      161
C                                                                      SPEC      162
C*****    *****    *****    *****    *****   CHAPTER 5   ***** *     SPEC      163
C*****    *****    *****    *****    *****   CHAPTER 5   ***** *     SPEC      164
C                                                                      SPEC      165
C  CONVERGENCE CHECK...ALL MOLE NUMBER CORRECTIONS MUST BE .LT. 1.0 PCT SPEC      166
C                                                                      SPEC      167
  500 IF (ETA.LT.1.0D0) GO TO 550                                      SPEC      168
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      DO 510 I=1,NS                                                          SPEC     169
      IF (DABS(X(I)).GT.0.0100) GO TO 590                                    SPEC     170
  510 CONTINUE                                                               SPEC     171
      LCONVG=.TRUE.                                                          SPEC     172
      HSUBO=HSUM*RGAS*TK                                                     SPEC     173
      RETURN                                                                 SPEC     174
C                                                                            SPEC     175
  590 CONTINUE                                                               SPEC     176
C                                                                            SPEC     177
C                                                                            SPEC     178
      RETURN                                                                 SPEC     179
C                                                                            SPEC     180
C******      ******      ******      ******      CHAPTER 6    ******       SPEC     181
C******      ******      ******      ******      CHAPTER 6    ******       SPEC     182
C                                                                            SPEC     183
      ENTRY ERATIO                                                           SPEC     184
C                                                                            SPEC     185
C   CALCULATES FUEL/AIR EQUIV RATIO, GIVEN MOLE NUMBERS IN S1 ARRAY,         SPEC     186
C   USING POSITIVE AND NEGATIVE OXIDATION STATES (VALENCES)                  SPEC     187
C                                                                            SPEC     188
      VP=0.000                                                               SPEC     189
      VM=0.000                                                               SPEC     190
      DO 610 I=1,NS                                                          SPEC     191
      IF (S1(I).LE.TINY) GO TO 610                                           SPEC     192
      DO 600 L=1,NLM                                                         SPEC     193
      IF (AL(L,I).EQ.0.00) GO TO 600                                         SPEC     194
      IF (ATOM(3,L).GT.0.000) VP=VP+AL(L,I)*ATOM(3,L)*S1(I)                  SPEC     195
      IF (ATOM(3,L).LT.0.000) VM=VM+AL(L,I)*ATOM(3,L)*S1(I)                  SPEC     196
  600 CONTINUE                                                               SPEC     197
  610 CONTINUE                                                               SPEC     198
C                                                                            SPEC     199
      VM=-VM                                                                 SPEC     200
      IF (VM.LT.TINY) GO TO 620                                              SPEC     201
      IF (VP.LT.TINY) GO TO 630                                              SPEC     202
      ER=VP/VM                                                               SPEC     203
      RETURN                                                                 SPEC     204
C                                                                            SPEC     205
  620 ER=1000000.000                                                         SPEC     206
      RETURN                                                                 SPEC     207
C                                                                            SPEC     208
  630 ER=0.000                                                               SPEC     209
C                                                                            SPEC     210
  900 RETURN                                                                 SPEC     211
      END                                                                    SPEC     212
      SUBROUTINE CREKO                                                       CRKO       2
C                                                                            CRKO       3
      DOUBLE PRECISION AL,BO,CPSUM,EMV,ER,FQ,HSUBO,HSUM,HO,PA,PI,PPLN,       NOXX     372
     1 QO,Q1,Q2,Q3,Q4,RGAS,RGASIN,RHOP,SM,SMINV,SMW,SSAVE,SO,S1,S2,TK,       NOXXX     22
     2 TKINV,TLN,Z,SMO                                                       NOXXX     23
      DOUBLE PRECISION RX,RX2,TACT,TACT2,TEN,TEN2,X1,X2,CERO                 NOXX     373
      DOUBLE PRECISION X,Y                                                   NOXXX     25
      DOUBLE PRECISION AMOLE,B,DX,GF,PECWT,RTLN,SUM,SUMX,SUMY,SUM1,          NOXXX     26
     1 TENLN,TM1,TM2,T1,T2,XBAR,XMAX,XMIN,YBAR                               NOXXX     27
      LOGICAL LADIAB,LCONVG,LDEBUG,LEQUIL,LMOLES,LNRG,LREACT,LSI,LENER       NOXX     374
C                                                                            CRKO       6
      COMMON                                                                 CRKO       7
     3/CCHEMI/CPSUM,HSUM,FQ,PPLN,RGAS,RGASIN,SMINV,TKINV,TLN,LNRG            NOXX     375
     1/CEQUIL/AL(7,30),ATOM(3,7),BO(7),PI(7)                                 CRKO       9
     1/CINDEX/IDCO,IDFU,IDO2,IDN2,IDH2O,IDCO2,IDH1,IDH2,IDN1,IDNO,IDNO2      NOXX     376
     1,IDO,IDOH,THCPS,ILC,ILH,IMAT,ITER,JJ,N1,N2,N3,NA,NGLOB,NGLOBP,         NOXX     377
     2 NLM,NO,NSM,NS1,NS2,IDCH                                               4STEP    605
     1/CMATRI/X(32),Y(32)                                                    NOXX     379
     1/CPARAM/ASUB(30,3),EMV,ER,HSUBO,NDEBUG,NS,PA,QO,Q1,Q2,Q3,Q4,RHOP,      CRKO      13
     1 SM,SMW(30),SMO,S1(30),S2(30),TK,LADIAB,LDEBUG,LEQUIL,LREACT,LENER     NOXX     380
```

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     2,EDKIJ,LCONVG                                                    NOXX     381
     1/CREACT/BX(36),BX2(36),ID(6,36),MOOR(36),TACT(36),TACT2(36),     CRKO      15
     2 TEN(36),TEN2(36),X1(36),X2(36),CEBU(36)                         NOXX     382
     1/CSPECE/HO(30),SO(30),SSAVE(30),Z(7,2,30)                        NOXX     383
C                                                                      CRKO      18
C*********************************************************************** CRKO    19
C  THIS SUBROUTINE IS THE INITIALIZING ROUTINE. THE FIRST CALL READS    CRKO      20
C  (1) ELEMENT DATA DECK, (2) THERMO DATA DECK, AND (3) MECHANISM DATA  CRKO      21
C  DECK.  EACH SUBSEQUENT CALL READS ONE REACTANTS DATA DECK...NO LIMIT CRKO      22
C  ON NUMBER OF CALLS...ONE FOR EACH DIFFERENT REACTANT STREAM          CRKO      23
C  PRESSURE AND TEMPERATURE OF EACH REACTANT STREAM MUST BE SUPPLIED BY CRKO      24
C  CALLING PROGRAM IN PA AND TK, RESPECTIVELY                          CRKO      25
C  ON RETURN, CALLING PROGRAM MUST STORE MOLE NUMBERS S2(I), PRESSURE,  CRKO      26
C  TEMPERATURE, ENTHALPY AND DENSITY AT APPROPRIATE INLET GRID NODE     CRKO      27
C  REFERENCE  CREK    (WASHINGTON STATE UNIVERSITY)  MARCH 1976         CRKO      28
C*********************************************************************** CRKO    29
C                                                                      CRKO      30
      DIMENSION CDATA(12),AT(4),B(4)                                   CRKO      31
C                                                                      CRKO      32
      DATA ACO/4HCO  /,ACO2/4HCO2 /,AH2/4HH2  /,AH2O/4HH2O /,          CRKO      33
     1ANCH/4HMECH/,AN2/4HN2  /,AO2/4HO2  /,BLANK/4H    /,BLNK/2H  /,   CRKO      34
     2ELEM/4HELEM/,GAZ/1HG/,GLOB/4HGLOB/,NOL/1HM/,NSTRM/0/,           CRKO      35
     3REAC/4HREAC/,REVE/4HREVE/,TENLN/2.3025850930D0/,THER/4HTHER/,    CRKO      36
     4THIRD/4HM   /,XMAX/0.001D0/,XMIN/0.000333333D0/                 CRKO      37
      DATA CARB,CGS,COMM,HYDR/1HC,4HCGS ,4HCOMM,1HH/                   CRKO      38
C                                                                      CRKO      39
   10 READ(5,20) (CDATA(I),I=1,12)                                     CRKO      40
   20 FORMAT(12A4)                                                     CRKO      41
      WRITE(6,30) (CDATA(I),I=1,12)                                    CRKO      42
   30 FORMAT(1HO,5X,12A4)                                              CRKO      43
C                                                                      CRKO      44
      IF (CDATA(1).EQ.BLANK) GO TO 10                                  CRKO      45
      IF (CDATA(1).EQ.ELEM) GO TO 100                                  CRKO      46
      IF (CDATA(1).EQ.THER) GO TO 200                                  CRKO      47
      IF (CDATA(1).EQ.ANCH) GO TO 300                                  CRKO      48
      IF (CDATA(1).EQ.REAC) GO TO 400                                  CRKO      49
      GO TO 10                                                         CRKO      50
C                                                                      CRKO      51
C* * * * * * * * * * * * * * * * * * * * * CHAPTER 1 * * * * * * * * * CRKO    52
C* * * * * * * * * * * * * * * * * * * * * CHAPTER 1 * * * * * * * * * CRKO    53
C                                                                      CRKO      54
C  ***ELEMENTS***                                                      CRKO      55
C  READ ELEMENT DATA FROM CARDS                                        CRKO      56
C  ATOM(1,K) = SYMBOL, ATOM(2,K) = ATOMIC WT, ATOM(3,K) = VALENCE      CRKO      57
C                                                                      CRKO      58
  100 RGAS=8314.400                                                    CRKO      59
      RGASIN=1.0D0/RGAS                                                CRKO      60
      IDCO =0                                                          CRKO      61
      IDCO2=0                                                          CRKO      62
      IDH2 =0                                                          CRKO      63
      IDH2O=0                                                          CRKO      64
      IDN2 =0                                                          CRKO      65
      IDO2 =0                                                          CRKO      66
      ILC=0                                                            CRKO      67
      ILH=0                                                            CRKO      68
      LADIAB=.TRUE.                                                    CRKO      69
      LDEBUG=.FALSE.                                                   CRKO      70
      NDEBUG=5                                                         CRKO      71
      LEQUIL=.FALSE.                                                   NOXX     384
      LREACT=.TRUE.                                                    CRKO      73
      LSI=.TRUE.                                                       CRKO      74
      LNRG=.TRUE.                                                      NOXX     385
      LENER=.TRUE.                                                     NOXX     386
      SO=1.000                                                         CRKO      76
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C                                                                       CRKD      77
      NLM=1                                                             CRKD      78
  110 READ(5,120) (ATOM(K,NLM),K=1,3)                                   CRKD      79
  120 FORMAT(A2,7X,2F10.6)                                              CRKD      80
      IF (ATOM(1,NLM).EQ.BLANK) GO TO 140                               CRKD      81
      WRITE(6,130) (ATOM(K,NLM),K=1,3)                                  CRKD      82
  130 FORMAT(1X,A2,5X,2F15.6/)                                          CRKD      83
      IF (ATOM(1,NLM).EQ.CARB) ILC=NLM                                  CRKD      84
      IF (ATOM(1,NLM).EQ.HYDR) ILH=NLM                                  CRKD      85
      NLM=NLM+1                                                         CRKD      86
      GO TO 110                                                         CRKD      87
C                                                                       CRKD      88
  140 CONTINUE                                                          CRKD      89
      NLM=NLM-1                                                         CRKD      90
      N1=NLM+1                                                          CRKD      91
      N2=NLM+2                                                          CRKD      92
      N3=NLM+3                                                          CRKD      93
      GO TO 10                                                          CRKD      94
C                                                                       CRKD      95
C**  **  **  **  **  **  **  **  **  **  **  **  **  CHAPTER 2  **  **  **  CRKD      96
C**  **  **  **  **  **  **  **  **  **  **  **  **  CHAPTER 2  **  **  **  CRKD      97
C                                                                       CRKD      98
C  ***THERMO***                                                         CRKD      99
C  READ THERMODYNAMIC DATA CARDS                                        CRKD     100
C                                                                       CRKD     101
  200 NS=1                                                              CRKD     102
  201 READ(5,210) (CDATA(I),I=1,3),DT1,DT2,(AT(J),B(J),J=1,4),PHAZ,     CRKD     103
     1T1,T2,NCD                                                         CRKD     104
  210 FORMAT(3A4,6X,2A3,4(A2,F3.0),A1,2F10.3,I15)                       CRKD     105
      IF (CDATA(1).EQ.BLANK) GO TO 260                                  CRKD     106
      WRITE(6,211)(CDATA(I),I=1,3),DT1,DT2,(AT(J),B(J),J=1,4),PHAZ,     CRKD     107
     1T1,T2,NCD                                                         CRKD     108
  211 FORMAT(10X,3A4,6X,2A3,2X,4(A2,2X,F3.0),2X,A1,2X,2F10.3,I15)       CRKD     109
      IF (PHAZ.NE.GAZ) WRITE(6,212) (CDATA(I),I=1,3),PHAZ               CRKD     110
  212 FORMAT(1HO,10X,26HWARNING...DATA FOR SPECIES,2X,3A4,3X,           CRKD     111
     a11HNOT GAS BUT,2X,A1//)                                           CRKD     112
C-----READ Z WITH FIRST AND SECOND SUBSCRIPTS REVERSED                  CRKD     113
      READ(5,213) (Z(J,1,NS),J=1,5),NCD                                 CRKD     114
  213 FORMAT(5D15.8,I5)                                                 CRKD     115
      WRITE(6,214) (Z(J,1,NS),J=1,5),NCD                                CRKD     116
  214 FORMAT(10X,5D15.8,I5)                                             CRKD     117
      READ(5,213) (Z(J,1,NS),J=6,7),(Z(K,2,NS),K=1,3),NCD               CRKD     118
      WRITE(6,214) (Z(J,1,NS),J=6,7),(Z(K,2,NS),K=1,3),NCD              CRKD     119
      READ(5,215) (Z(J,2,NS),J=4,7),NCD                                 CRKD     120
  215 FORMAT(4D15.8,I20)                                                CRKD     121
      WRITE(6,216) (Z(J,2,NS),J=4,7),NCD                                CRKD     122
  216 FORMAT(10X,4D15.8,I20/)                                           CRKD     123
C                                                                       CRKD     124
C-----ESTABLISH ATOM STOICHIOMETRY...AL(L,N) = (KG-ATOMS ELEMENT L      CRKD     125
C-----PER KG-MOLECULE OF SPECIES N)                                     CRKD     126
C                                                                       CRKD     127
      DO 220 L=1,NLM                                                    CRKD     128
  220 AL(L,NS)=0.0D0                                                    CRKD     129
C                                                                       CRKD     130
      SUM=0.0D0                                                         CRKD     131
      DO 240 K=1,4                                                      CRKD     132
      IF (B(K).EQ.0.0D0) GO TO 240                                      CRKD     133
      DO 230 L=1,NLM                                                    CRKD     134
      IF (ATOM(1,L).NE.AT(K)) GO TO 230                                 CRKD     135
      AL(L,NS)=AL(L,NS)+B(K)                                            CRKD     136
C                                                                       CRKD     137
C-----ESTABLISH MOLECULAR WEIGHT OF SPECIES                             CRKD     138
C                                                                       CRKD     139
      SUM=SUM+ATOM(2,L)*B(K)                                            CRKD     140
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  230 CONTINUE                                                          CRKD    141
  240 CONTINUE                                                          CRKD    142
      SMW(NS)=SUM                                                       CRKD    143
      S2(NS)=1.0D-6                                                     CRKD    144
C                                                                       CRKD    145
C-----STORE HOLLERITH NAME OF SPECIES                                   CRKD    146
C                                                                       CRKD    147
      DO 250 I=1,3                                                      CRKD    148
  250 ASUB(NS,I)=CDATA(I)                                               CRKD    149
C                                                                       CRKD    150
C-----STORE INDEX NUMBER OF SPECIES                                     CRKD    151
C                                                                       CRKD    152
      IF (ASUB(NS,1).EQ.ACO)  IDCO=NS                                   CRKD    153
      IF (ASUB(NS,1).EQ.ACO2) IDCO2=NS                                  CRKD    154
      IF (ASUB(NS,1).EQ.AH2)  IDH2=NS                                   CRKD    155
      IF (ASUB(NS,1).EQ.AH2O) IDH2O=NS                                  CRKD    156
      IF (ASUB(NS,1).EQ.AN2)  IDN2=NS                                   CRKD    157
      IF (ASUB(NS,1).EQ.AO2)  IDO2=NS                                   CRKD    158
      IF(NS.NE.IDCH)GO TO 252                                           4STEP   606
      DO 251 I=1,2                                                      4STEP   607
      DO 251 J=1,7                                                      4STEP   608
  251 Z(J,I,IDCH)=Z(J,I,LDCH)*(SMW(IOFU)-2.000)/28.000                  4STEP   609
  252 CONTINUE                                                          4STEP   610
C                                                                       CRKD    159
      NS=NS+1                                                           CRKD    160
      GO TO 201                                                         CRKD    161
C                                                                       CRKD    162
  260 NS=NS-1                                                           CRKD    163
      NSM=NS+1                                                          CRKD    164
      NQ=NS+2                                                           CRKD    165
      NA=NS+3                                                           CRKD    166
      GO TO 10                                                          CRKD    167
C                                                                       CRKD    168
C***   ***   ***   ***   ***   ***   ***   ***   CHAPTER 3   ***   ***  CRKD    169
C***   ***   ***   ***   ***   ***   ***   ***   CHAPTER 3   ***   ***  CRKD    170
C                                                                       CRKD    171
C  ***MECHANISM***                                                      CRKD    172
C  READ MECHANISM/RATE DATA CARDS                                       CRKD    173
C  THE VARIABLE DT1 (COLUMNS 73/76) IS USED AS A FLAGG                  CRKD    174
C  CGS  ---  CGS UNITS, RATE CONSTANTS IN GM-MOLES, CM, SEC             CRKD    175
C            AND EACT IN (KCAL/GM-MOLE)                                 CRKD    176
C  COMM ---  COMMENT CARD, FIRST 48 CHARACTERS PRINTED OUT              CRKD    177
C  REVF ---  REVERSE RATE DATA, IN SAME UNITS AS FORWARD DATA           CRKD    178
C  GLOB ---  GLOBAL RATE EXPRESSION DATA IN SI UNITS                    CRKD    179
C  OTHERWISE THE SI UNITS (KG-MOLES, M, SEC) ARE ASSUMED                CRKD    180
C  DT1 AND DT2 (COL 73/80) CAN HAVE ANYTHING (COMMENTS) IF ABOVE FOUR   CRKD    181
C  WORDS ARE NOT REQUIRED                                               CRKD    182
C  TACT IS ACTIVATION TEMPERATURE, = EACT/GASCON, DEG K                 CRKD    183
C                                                                       CRKD    184
  300 JJ=1                                                              CRKD    185
      NGLOB=0                                                           CRKD    186
C                                                                       CRKD    187
  310 READ(5,311)(CDATA(I),I=1,12),BX(JJ),TEN(JJ),TACT(JJ),             NOXX    387
     1 CFRU(JJ),DT1,DT2                                                 NOXX    388
  311 FORMAT(12A4,F7.3,F5.3,F7.3,F5.3,2A4)                              NOXX    389
      IF (CDATA(1).EQ.BLANK.AND.DT1.NE.COMM) GO TO 356                  CRKD    190
C-----CHECK FOR COMMENT CARD                                            CRKD    191
      IF (DT1.NE.COMM) GO TO 313                                        CRKD    192
      WRITE(6,312) (CDATA(I),I=1,12)                                    CRKD    193
  312 FORMAT(1HO,5X,3H***,12A4,3H***)                                   CRKD    194
      GO TO 310                                                         CRKD    195
C-----CHECK FOR REVERSE RATE DATA...ORDER OF CARDS MUST BE CORRECT      CRKD    196
C-----UNITS OF REVERSE DATA ASSUMED SAME AS FORWARD DATA                CRKD    197
  313 IF (DT1.NE.REVF) GO TO 315                                        CRKD    198
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      J=JJ-1                                                            CRKD    199
      BX2(J)=BX(JJ)                                                     CRKD    200
      TEN2(J)=TEN(JJ)                                                   CRKD    201
      TACT2(J)=TACT(JJ)                                                 CRKD    202
      WRITE(6,314) BX2(J),TEN2(J),TACT2(J),DT1,DT2                      CRKD    203
  314 FORMAT(14X,17HREVERSE RATE DATA,28X,3F15.3,2A4)                   CRKD    204
C-----CONVERT BX2 FOR INTERNAL CALCULATIONS                             CRKD    205
      BX2(J)=BX2(J)*TENLN                                               CRKD    206
      IF (LSI) GO TO 310                                                CRKD    207
      BX2(J)=BX2(J)-TENLN*3.000                                         CRKD    208
      TACT2(J)=TACT2(J)*1000.000/1.987D0                                CRKD    209
      IF (MODR(J).EQ.2) BX2(J)=BX2(J)-TENLN*3.000                       CRKD    210
      GO TO 310                                                         CRKD    211
C-----CHECK FOR UNITS                                                   CRKD    212
  315 LSI=.TRUE.                                                        CRKD    213
      IF (DT1.EQ.CGS) LSI=.FALSE.                                       CRKD    214
C                                                                       CRKD    215
      WRITE(6,316) JJ,(CDATA(I),I=1,12),BX(JJ),TEN(JJ),TACT(JJ),DT1,DT2 CRKD    216
  316 FORMAT(1HO,5X,I5,4H.   ,12A4,3F15.3,5X,2A4)                       CRKD    217
      IF (.NOT. LSI) TACT(JJ)=TACT(JJ)*1000.D0/1.987D0                  CRKD    218
      IF (DT1.EQ.GLOB) NGLOB=NGLOB+1                                    CRKD    219
C-----CONVERT BX FOR INTERNAL CALCULATIONS                              CRKD    220
      BX(JJ)=BX(JJ)*TENLN                                               CRKD    221
C                                                                       CRKD    222
C-----ID(I,J) IS THE INDEX NUMBER OF THE I-TH DISTINCT SPECIES IN       CRKD    223
C-----REACTION J ... I=1,4 AS NO DISTINCT THIRD BODIES ARE CONSIDERED   CRKD    224
C                                                                       CRKD    225
      DO 320 I=1,6                                                      CRKD    226
  320 ID(I,JJ)=0                                                        CRKD    227
C                                                                       CRKD    228
      DO 325 N=1,6                                                      CRKD    229
      K=N*2-1                                                           CRKD    230
      IF (CDATA(K).EQ.BLANK) GO TO 325                                  CRKD    231
      IF (CDATA(K).NE.THIRD) GO TO 321                                  CRKD    232
      CDATA(K)=BLANK                                                    CRKD    233
      GO TO 325                                                         CRKD    234
  321 CONTINUE                                                          CRKD    235
      DO 322 I=1,NS                                                     CRKD    236
      IF (CDATA(K).NE.ASUB(I,1)) GO TO 322                              CRKD    237
      IF (CDATA(K+1).NE.ASUB(I,2)) GO TO 322                            CRKD    238
      II=I                                                              CRKD    239
      GO TO 323                                                         CRKD    240
  322 CONTINUE                                                          CRKD    241
  323 CONTINUE                                                          CRKD    242
      ID(N ,JJ)=II                                                      CRKD    243
  325 CONTINUE                                                          CRKD    244
C                                                                       CRKD    245
C                                                                       CRKD    246
C-----STORE THE TYPE OF REACTION...THREE TYPES                          CRKD    247
C     MODR 1 ...A + B (+C) ---) D + E (+F)                              CRKD    248
C     MODR 2 ... AB + M ---  A + B + M                                  CRKD    249
C     MODR 3 ... A + B + M ---  AB + M                                  CRKD    250
C                                                                       CRKD    251
      MODR(JJ)=1                                                        CRKD    252
      IF (ID(2,JJ).EQ.0) MODR(JJ)=2                                     CRKD    253
      IF (ID(5,JJ).EQ.0) MODR(JJ)=3                                     CRKD    254
C                                                                       CRKD    255
C                                                                       CRKD    256
C     THE FOLLOWING SECTION, UP TO STATEMENT 355 INCLUSIVE, MAY BE      CRKD    257
C     ELIMINATED IF REVERSE (AS WELL AS FORWARD) RATE DATA IS SUPPLIED  CRKD    258
C     FOR  ** ALL ** REACTIONS.                                         CRKD    259
C                                                                       CRKD    260
C     CALCULATES REVERSE RATE CONSTANTS FROM EQUILIBRIUM CONSTANTS      CRKD    261
C     AND FORWARD RATE CONSTANTS FOR FIFTEEN POINTS                     CRKD    262
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C      OVER THE TEMPERATURE RANGE 1000 TO 3000 DEG K                    CRKD     263
C                                                                       CRKD     264
C      INSERTED 1 STEP (M.D.HOOVEN, 7/22/79)                            CRKD     265
       IF (DT1.EQ.GLOB) GO TO 357                                       CRKD     266
       IF (DT1.EQ.GLOB) GO TO 355                                       CRKD     267
       DX=(XMAX-XMIN)/14.CDO                                            CRKD     268
       SUMX=0.000                                                       CRKD     269
       SUMY=0.000                                                       CRKD     270
       IHCPS=2                                                          CRKD     271
       DO 351 N=1,15                                                    CRKD     272
       X(N)=XMIN+DX*FLOAT(N-1)                                          NOXXX     28
       SUMX=SUMX+X(N)                                                   CRKD     274
       TKINV=X(N)                                                       CRKD     275
       TK=1.000/TKINV                                                   CRKD     276
       TLN=DLOG(TK)                                                     CRKD     277
       NS1=1                                                            NOXX     390
       NS2=NS                                                           NOXX     391
       CALL HCPS                                                        CRKD     278
       SUM1=0.000                                                       CRKD     279
       DO 350 ND=1,6                                                    CRKD     280
       K=ID(ND,JJ)                                                      CRKD     281
       IF (K.EQ.0) GO TO 350                                            CRKD     282
       GF=HO(K)-SO(K)                                                   CRKD     283
       IF (ND.LT.4) SUM1=SUM1+GF                                        CRKD     284
       IF (ND.GE.4) SUM1=SUM1-GF                                        CRKD     285
  350 CONTINUE                                                          CRKD     286
       TM1=0.CDO                                                        CRKD     287
C     NATURAL LOGS OF GAS CONSTANTS...R=82.057 CM3-ATM/GMOL,K (CGS)     CRKD     288
C       AND R=C.082057 M3-ATM/KGMOL,K (SI)                             CRKD     289
       RTLN=TLN+4.4074DC                                                CRKD     290
       IF (LSI) RTLN=TLN-2.5003400                                      CRKD     291
       IF (NDDR(JJ).GT.1) GO TO 3501                                    CRKD     292
       IF (ID(3,JJ).EQ.0) TM1=TM1+RTLN                                  CRKD     293
       IF (ID(6,JJ).EQ.0) TM1=TM1-RTLN                                  CRKD     294
       GO TO 3502                                                       CRKD     295
 3501 CONTINUE                                                          CRKD     296
       IF (ID(2,JJ).EQ.0) TM1=RTLN                                      CRKD     297
       IF (ID(5,JJ).EQ.0) TM1=-RTLN                                     CRKD     298
 3502 CONTINUE                                                          CRKD     299
       Y(N)=TM1-SUM1+TEN(JJ)*TLN-TACT(JJ)*TKINV+BX(JJ)                  CRKD     300
       SUMY=SUMY+Y(N)                                                   CRKD     301
  351 CONTINUE                                                          CRKD     302
       XBAR=SUMX/15.000                                                 CRKD     303
       YBAR=SUMY/15.CDO                                                 CRKD     304
       SUMX=0.000                                                       CRKD     305
       SUM1=C.000                                                       CRKD     306
       SUMY=0.CDC                                                       CRKD     307
       DO 352 N=1,15                                                    CRKD     308
       SUMX=SUMX+Y(N)*(X(N)-XBAR)                                       CRKD     309
       SUM1=SUM1+(X(N)-XBAR)**2                                         CRKD     310
       SUMY=SUMY+(Y(N)-YBAR)**2                                         CRKD     311
  352 CONTINUE                                                          CRKD     312
       TEN2(JJ)=0.000                                                   CRKD     313
       TACT2(JJ)=-SUMX/SUM1                                             CRKD     314
       BX2(JJ)=(YBAR+TACT2(JJ)*XBAR)/TENLN                              CRKD     315
       SUMX=0.000                                                       CRKD     316
       DO 353 N=1,15                                                    CRKD     317
       SUMX=SUMX+(Y(N)+TACT2(JJ)*X(N)-TENLN*BX2(JJ))**2                 CRKD     318
  353 CONTINUE                                                          CRKD     319
       SUMY=DSQRT(1.000-SUMX/SUMY)                                      CRKD     320
       SUMX=DSQRT(SUMX/14.000)                                          CRKD     321
       CDATA(1)=TACT2(JJ)                                               CRKD     322
       IF (.NOT.LSI) CDATA(1)=TACT2(JJ)*1.98700*0.001DC                 CRKD     323
       WRITE(6,354) BX2(JJ),TEN2(JJ),CDATA(1),SUMX,SUMY                 CRKD     324
```

```
  354 FORMAT(6X,57H CALCULATED REVERSE RATE DATA, STD DEV AND CORR COEF  CRKD  325
     1 =    ,3F15.3,4X,1P2D10.3)                                       CRKD  326
C-----CONVERT BX2 FOR INTERNAL CALCULATIONS                           CRKD  327
      BX2(JJ)=BX2(JJ)*TENLN                                           CRKD  328
C                                                                     CRKD  329
C-----SET REVERSE REACTION RATE VARIABLES=0 FOR GLOBAL REACTIONS      CRKD  330
C-----SO THAT THESE VARIABLES ARE DEFINED FOR THE KINETIC RATE        CRKD  331
C-----PRINTOUT (M.D.HOOVEN 7/22/79)                                   CRKD  332
  357 IF (DT1.NE.GLOB) GO TO 355                                      CRKD  333
      TACT2(JJ)=C                                                     CRKD  334
      TEN2(JJ)=0                                                      CRKD  335
      BX2(JJ)=0                                                       CRKD  336
  355 JJ=JJ+1                                                         CRKD  337
C-----CONVERT ALL RATE DATA TO SI UNITS                               CRKD  338
      IF (LSI) GO TO 310                                              CRKD  339
      J=JJ-1                                                          CRKD  340
      BX(J)=BX(J)-TENLN*3.0D0                                         CRKD  341
      BX2(J)=BX2(J)-TENLN*3.0D0                                       CRKD  342
      IF (MODR(J).EQ.2) BX2(J)=BX2(J)-TENLN*3.0D0                     CRKD  343
      IF (MODR(J).EQ.3) BX(J)=BX(J)-TENLN*3.0D0                       CRKD  344
      IF (MODR(J).NE.1) GO TO 310                                     CRKD  345
      IF (ID(3,J).NE.0) BX(J)=BX(J)-TENLN*3.0D0                       CRKD  346
      IF (ID(6, J).NE.0) BX2(J)=BX2(J)-TENLN*3.0D0                    CRKD  347
      GO TO 310                                                       CRKD  348
C                                                                     CRKD  349
  356 JJ=JJ-1                                                         CRKD  350
      NGLOBP=NGLOB+1                                                  CRKD  351
C                                                                     CRKD  352
C-----PRINT OUT ARRAY OF STOICHIOMETRIC COEFFICIENTS                  CRKD  353
C                                                                     CRKD  354
      DO 372 J=1,JJ                                                   CRKD  355
      DO 370 N=1,6                                                    CRKD  356
      K=N*2-1                                                         CRKD  357
      L=N                                                             CRKD  358
      CDATA(K)=BLANK                                                  CRKD  359
      CDATA(K+1)=BLANK                                                CRKD  360
      IDLJ=ID(L,J)                                                    CRKD  361
      IF (IDLJ.EQ.0) GO TO 370                                        CRKD  362
      CDATA(K)=ASUB(IDLJ,1)                                           CRKD  363
      CDATA(K+1)=ASUB(IDLJ,2)                                         CRKD  364
  370 CONTINUE                                                        CRKD  365
      IF (ID(2,J).EQ.0) CDATA(5)=THIRD                                CRKD  366
      IF (ID(5,J).EQ.0) CDATA(5)=THIRD                                CRKD  367
      IF (MODR(J).GT.1) CDATA(11)=THIRD                               CRKD  368
      WRITE(6,371) J,(CDATA(K),K=1,12)                                CRKD  369
  371 FORMAT(5X,I5,1H.,5X,6A4,/H----- ,6X,6A4/)                       CRKD  370
  372 CONTINUE                                                        CRKD  371
C                                                                     CRKD  372
C-----PRINT OUT ALL RATE DATA IN SI UNITS                             CRKD  373
C                                                                     CRKD  374
      WRITE(6,380)                                                    CRKD  375
  380 FORMAT(//1HO,40X,29HKINETIC RATE DATA IN SI UNITS/              CRKD  376
     A1HO,6X,1HJ,2X,4HMODR,16X,2HID,19X,2HBX,10X,3HTEN,9X,4HTACT,     CRKD  377
     B13X,3HBX2,9X,4HTEN2,9X,5HTACT2/)                                CRKD  378
      DO 382 J=1,JJ                                                   CRKD  379
      TM1=BX(J)/TENLN                                                 CRKD  380
      TM2=BX2(J)/TENLN                                                CRKD  381
      WRITE(6,381) J,MODR(J),(ID(I,J),I=1,6),TM1,TEN(J),TACT(J),      CRKD  382
     1TM2,TEN2(J),TACT2(J)                                            CRKD  383
  382 CONTINUE                                                        CRKD  384
  381 FORMAT((5X,I2,1H.,I4,3X,6I4,2(3X,3F13.3)))                      CRKD  385
C                                                                     CRKD  386
C-----SET CONTACT INDEXES TO UNITY                                    CRKD  387
      DO 390 J=1,JJ                                                   CRKD  388
```

```
      X1(J)=1.000                                                       CRKD    389
      X2(J)=1.000                                                       CRKD    390
  390 CONTINUE                                                          CRKD    391
C                                                                       CRKD    392
      RETURN                                                            CRKD    393
C                                                                       CRKD    394
C****     ****     ****     ****     ****     ****     CHAPTER 4   ****  ***  CRKD    395
C****     ****     ****     ****     ****     ****     CHAPTER 4   ****  ***  CRKD    396
C                                                                       CRKD    397
C  ***REACTANTS***                                                     CRKD    398
C  READ REACTANTS DATA CARDS FOR EACH INLET STREAM                      CRKD    399
C                                                                       CRKD    400
  400 NSTRM=NSTRM+1                                                     CRKD    401
      LMOLES=.FALSE.                                                    CRKD    402
C-----SCRUB SPECIES MOLE NUMBER ARRAY                                   CRKD    403
      DO 405 I=1,NS                                                     CRKD    404
  405 S2(I)=0.000                                                       CRKD    405
      SUM1=0.000                                                        CRKD    406
C                                                                       CRKD    407
  410 READ(5,411) (AT(I),B(I),I=1,4),(COATA(I),I=1,2),PECWT,MOLE,PHAZ   CRKD    408
  411 FORMAT(4(A2,F7.5),2A4,1X,F7.5,A1,9X,A1)                           CRKD    409
      IF (AT(1).EQ.BLNK) GO TO 450                                      CRKD    410
      WRITE(6,412) (AT(I),B(I),I=1,4),(COATA(I),I=1,2),PECWT,MOLE,      CRKD    411
     1PHAZ,NSTRM                                                        CRKD    412
  412 FORMAT(1X,4(2X,A2,F9.5),2X,2A4,2X,F9.5,2X,A1,2X,A1,2X,I5)         CRKD    413
      IF (MOLE.EQ.MOL) LMOLES=.TRUE.                                    CRKD    414
C                                                                       CRKD    415
C-----ESTABLISH MOLE NUMBERS (KG-MOL I/KGM MIXTURE) IN INLET STREAM     CRKD    416
C                                                                       CRKD    417
      TKINV=1.000/TK                                                    CRKD    418
C     SCREEN FOR CONDENSED SPECIES                                      CRKD    419
      DO 430 I=1,NS                                                     CRKD    420
C-----SCREEN FOR SPECIES NAME                                           CRKD    421
      IF (COATA(1).NE.ASUB(I,1)) GO TO 430                              CRKD    422
      IF (COATA(2).NE.ASUB(I,2)) GO TO 430                              CRKD    423
      DO 420 L=1,NLM                                                    CRKD    424
C-----SCREEN FOR ATOMIC COMPOSITION                                     CRKD    425
      DO 420 K=1,4                                                      CRKD    426
      IF (ATOM(I,L).NE.AT(K)) GO TO 420                                 CRKD    427
      IF (AL(L,I).NE.B(K)) GO TO 430                                    CRKD    428
  420 CONTINUE                                                          CRKD    429
C-----IF PECWT IS RELATIVE MASS, CONVERT TO RELATIVE MOLE NUMBERS       CRKD    430
      AMOLE=PECWT/SMW(I)                                                CRKD    431
      IF (LMOLES) AMOLE=PECWT                                           CRKD    432
      S2(I)=S2(I)+AMOLE                                                 CRKD    433
      SUM1=SUM1+AMOLE*SMW(I)                                            CRKD    434
      GO TO 410                                                         CRKD    435
  430 CONTINUE                                                          CRKD    436
C                                                                       CRKD    437
      WRITE(6,440)                                                      CRKD    438
  440 FORMAT(1HO,10X,45H REACTANT ABOVE NOT FOUND IN THERMO LIBRARY/ )   CRKD    439
      GO TO 410                                                         CRKD    440
C                                                                       CRKD    441
  450 CONTINUE                                                          CRKD    442
C                                                                       CRKD    443
C-----ESTABLISH MIXTURE ENTHALPY                                        CRKD    444
C                                                                       CRKD    445
      IHCPS=1                                                           CRKD    446
      CALL HCPS                                                         CRKD    447
C                                                                       CRKD    448
      WRITE(6,460) NSTRM                                                CRKD    449
  460 FORMAT(1HO,19H*** REACTANT STREAM,I3,4H ***/                      CRKD    450
     A1HO,5X,1HI,4X,7HSPECIES,14X,16HMOLECULAR WEIGHT,5X,               CRKD    451
     B12HMOLE NUMBERS,8X,14HMASS FRACTIONS/32X,17H(KG-MOLE I)/(KG I),   CRKD    452
```

```
     C4X,17H(KGMOLE I)/(KG X),9X,13H(KG I)/(KG X)/)                    CRKO     453
      HSUM=0.0D0                                                       CRKO     454
      SM=0.0D0                                                         CRKO     455
      DO 480 I=1,NS                                                    CRKO     456
      S2(I)=S2(I)/SUM1                                                 CRKO     457
C-----S2(I) IN MOLE NUMBERS, KG-MOLES I/KG MIXTURE                     CRKO     458
      HSUM=HSUM+HO(I)*S2(I)                                            CRKO     459
      SM=SM+S2(I)                                                      CRKO     460
      DT1=S2(I)*SMW(I)                                                 CRKO     461
      WRITE(6,470) I,(ASUB(I,J),J=1,3),SMW(I),S2(I),DT1                CRKO     462
  470 FORMAT(5X,I2,1H.,4X,3A4,1P3D20.3)                                CRKO     463
  480 CONTINUE                                                         CRKO     464
C-----HSUBO IN JOULES/KG REACTANT MIXTURE                              CRKO     465
      HSUBO=HSUM*RGAS*TK                                               CRKO     466
C-----RHOP IS MASS DENSITY, KG/CU M                                    CRKO     467
      RHOP=PA/(RGAS*TK*SM)                                             CRKO     468
C                                                                      CRKO     469
      SMINV=1.0D0/SM                                                   CRKO     470
      WRITE(6,490) TK,HSUBO,PA,RHOP,SMINV                              CRKO     471
  490 FORMAT(1HC//12X,13HTEMPERATURE =,1PD12.3,3X,5HDEG K/             CRKO     472
     A12X,10HENTHALPY =,3X,1PD12.3,3X,9HJOULES/KG/                     CRKO     473
     B12X,10HPRESSURE =,3X,1PD12.3,3X,6HN/M**2/                        CRKO     474
     C12X,9HDENSITY =,4X,1PD12.3,3X,7HKG/M**3/                         CRKO     475
     D12X,13HMEAN MOL WT =,1PD12.3,3X,9HKG/KGMOLE//)                   CRKO     476
C                                                                      CRKO     477
C-----ON RETURN, CALLING PROGRAM MUST STORE MOLE NUMBERS S2(I),        CRKO     478
C-----PRESSURE, TEMPERATURE, ENTHALPY AND DENSITY AT APPROPRIATE INLET CRKO     479
C-----INLET GRID NODE                                                  CRKO     480
C                                                                      CRKO     481
      RETURN                                                           CRKO     482
      END                                                              CRKO     483
      SUBROUTINE HCPS                                                  HCPS       2
C *** MODIFIED FOR CONDENSED SPECIES 7-79 D.T.PRATT                    HCPS       3
C                                                                      HCPS       4
      DOUBLE PRECISION CPSUM,EMV,ER,FQ,HSUBO,HSUM,HO,PA,PPLN,          NOXX     392
     1 QQ,Q1,Q2,Q3,Q4,RGAS,RGASIN,RHOP,SM,SMINV,SMW,SSAVE,SO,S1,S2,TK,  NOXXX     30
     2 TKINV,TLN,Z,SMO                                                 NOXXX     31
      DOUBLE PRECISION CP1,CP2,CP3,CP4,CP5,P2,P25,P333,P5,TKCU,TKSQ,TK4 NOXXX     32
      LOGICAL LADIAB,LCONVG,LDEBUG,LEQUIL,LNRG,LREACT,LENER             NOXX     393
C                                                                      HCPS       7
      COMMON                                                           HCPS       8
     3/CCHEMI/CPSUM,HSUM,FQ,PPLN,RGAS,RGASIN,SMINV,TKINV,TLN,LNRG      NOXX     394
     1/CINDEX/IDCO,IOFU,IDO2,IDN2,IDH2O,IDCO2,IDH1,IDH2,IDN1,IDNO,IDNO2 NOXX     395
     1,IOO,IOOH,IHCPS,ILC,ILH,IMAT,ITER,JJ,N1,N2,N3,NA,NGLOB,NGLOBP,   NOXX     396
     2 NLM,NQ,NSM,NS1,NS2,IOCH                                         4STEP    611
     1/CPARAM/ASUB(30,3),EMV,ER,HSUBO,NDEBUG,NS,PA,QQ,Q1,Q2,Q3,Q4,RHOP, HCPS      12
     1 SM,SMW(30),SPO,S1(30),S2(30),TK,LADIAB,LDEBUG,LEQUIL,LREACT,LENER NOXX     396
     2,EOKIJ,LCONVG                                                    NOXX     399
     1/CSPECE/HO(30),SO(30),SSAVE(30),Z(420)                           NOXX     400
C                                                                      HCPS      15
C**********************************************************************HCPS      16
C  THIS SUBROUTINE CALCULATES THE NON-DIMENSIONAL, 1-ATM VALUES OF     HCPS      17
C  ENTHALPY, SPECIFIC HEAT, AND ENTROPY FOR A GIVEN VALUE OF TEMPERATURE HCPS      18
C  (DEG K)  THE Z ARRAY IS REFERENCED AS HAVING ONLY ONE SUBSCRIPT     HCPS      19
C  TO SAVE INTERNAL SUBSCRIPT CALCULATIONS.                           HCPS      20
C  Z(IC,IT,IS) ---  Z(IC+7*(IT-1)+2*(IS-1)) FOR Z(7,2,20)             HCPS      21
C  WHERE IC=1,7. COEF FOR TEMP RANGE IT=1 OR 2. FOR SPECIES IS=1,NS.  HCPS      22
C  NOTE THAT THE FIRST 2 SUBSCRIPTS ARE REVERSED FROM THE             HCPS      23
C  GORDON AND MCBRIDE PRACTICE                                        HCPS      24
C  REFERENCE  GORDON AND MCBRIDE  (NASA SP-273, 1971)                 HCPS      25
C**********************************************************************HCPS      26
C                                                                      HCPS      27
      DATA ICIT/14/                                                    HCPS      28
      DATA P2,P25,P333,P5/0.200,0.2500,0.333333300,0.500/              NOXXX     33
```

```
C                                                                       HCPS      30
      IT=0                                                              HCPS      31
      IF (TK.LT.1000.000) IT=7                                          HCPS      32
C                                                                       HCPS      33
      TKSQ=TK**2                                                        HCPS      34
      TKCU=TKSQ*TK                                                      HCPS      35
      TK4=TKCU*TK                                                       HCPS      36
      CPSUM=0.000                                                       HCPS      37
      GO TO (11,21,31,41),IHCPS                                         NOXX     401
C                                                                       HCPS      39
C-----IHCPS=1 ---  JUST CPSUM AND HO(I) REQUIRED                        HCPS      40
C                                                                       HCPS      41
   11 DO 10 I=NS1,NS2                                                   NOXX     402
      K=IT+ICIT*(I-1)                                                   HCPS      43
      CP1=Z(K+1)                                                        HCPS      44
      CP2=TK*Z(K+2)                                                     HCPS      45
      CP3=TKSQ*Z(K+3)                                                   HCPS      46
      CP4=TKCU*Z(K+4)                                                   HCPS      47
      CP5=TK4*Z(K+5)                                                    HCPS      48
      CPSUM=CPSUM+(CP1+CP2+CP3+CP4+CP5)*S2(I)                           HCPS      49
      HO(I)=P2*CP5+P25*CP4+P333*CP3+P5                                  HCPS      50
     X       *CP2+CP1+TKINV*Z(K+6)                                      HCPS      51
   10 CONTINUE                                                          HCPS      52
      RETURN                                                            HCPS      53
C                                                                       HCPS      54
C-----IHCPS=2 ---  CPSUM, HO(I) AND SO(I) REQUIRED                      HCPS      55
C                                                                       HCPS      56
   21 DO 30 I=NS1,NS2                                                   NOXX     403
      K=IT+ICIT*(I-1)                                                   HCPS      59
      CP1=Z(K+1)                                                        HCPS      60
      CP2=TK*Z(K+2)                                                     HCPS      61
      CP3=TKSQ*Z(K+3)                                                   HCPS      62
      CP4=TKCU*Z(K+4)                                                   HCPS      63
      CP5=TK4*Z(K+5)                                                    HCPS      64
      CPSUM=CPSUM+(CP1+CP2+CP3+CP4+CP5)*S2(I)                           HCPS      65
      HO(I)=P2*CP5+P25*CP4+P333*CP3+P5                                  HCPS      66
     X       *CP2+CP1+TKINV*Z(K+6)                                      HCPS      67
      SO(I)=P25*CP5+P333*CP4+P5*CP3                                     HCPS      68
     X        +CP2+TLN*CP1+Z(K+7)                                        HCPS      69
   30 CONTINUE                                                          HCPS      70
      RETURN                                                            HCPS      71
C-----IHCPS=3 ---  HSUM REQUIRED                                        NOXX     404
   31 HSUM=0.000                                                        NOXX     405
      DO 40 I=NS1,NS2                                                   NOXX     406
      K=IT+ICIT*(I-1)                                                   NOXX     407
      CP1=Z(K+1)                                                        NOXX     408
      CP2=TK*Z(K+2)                                                     NOXX     409
      CP3=TKSQ*Z(K+3)                                                   NOXX     410
      CP4=TKCU*Z(K+4)                                                   NOXX     411
      CP5=TK4*Z(K+5)                                                    NOXX     412
      HO(I)=P2*CP5+P25*CP4+P333*CP3+P5*CP2+CP1+TKINV*Z(K+6)             NOXX     413
      HSUM=HSUM+HO(I)*S2(I)                                             NOXX     414
   40 CONTINUE                                                          NOXX     415
      RETURN                                                            NOXX     416
C-----IHCPS=4 ---  HSUM AND CPSUM REQUIRED                              NOXX     417
   41 HSUM=0.000                                                        NOXX     418
      DO 50 I=NS1,NS2                                                   NOXX     419
      K=IT+ICIT*(I-1)                                                   NOXX     420
      CP1=Z(K+1)                                                        NOXX     421
      CP2=TK*Z(K+2)                                                     NOXX     422
      CP3=TKSQ*Z(K+3)                                                   NOXX     423
      CP4=TKCU*Z(K+4                                                    NOXX     424
      CP5=TK4*Z(K+5)                                                    NOXX     425
      CPSUM=CPSUM+(CP1+CP2+CP3+CP4+CP5)*S2(I)                           NOXX     426
```

```
      HO(I)=P2*CP5+P25*CP4+P333*CP3+P5*CP2+CP1+TKINV*Z(K+6)          NOXX      427
      HSUM=HSUM+HO(I)*S2(I)                                          NOXX      428
   50 CONTINUE                                                       NOXX      429
      RETURN                                                         NOXX      430
      END                                                            HCPS       72
```

APPENDIX E

LIST OF DEPENDENT VARIABLES

AND SOURCE TERMS

APPENDIX E

LIST OF DEPENDENT VARIABLES AND SOURCE TERMS

TABLE E-1

Dependent Variable	Source Term
u (axial velocity)	$\frac{\partial}{\partial x}\left(\mu_{eff}\frac{\partial u}{\partial x}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(\mu_{eff}\, r\frac{\partial v}{\partial x}\right) + \frac{1}{r}\frac{\partial}{\partial \theta}\left(\mu_{eff}\frac{\partial w}{\partial x}\right) + S^{u}_{spray} - \frac{\partial p}{\partial x}$
v (radial velocity)	$\frac{\partial}{\partial x}\left(\mu_{eff}\frac{\partial u}{\partial r}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(\mu_{eff}\, r\frac{\partial v}{\partial r}\right) + \frac{1}{r}\frac{\partial}{\partial \theta}\left[\mu_{eff}\left(\frac{\partial w}{\partial r} - \frac{w}{r}\right)\right] - 2\frac{\mu_{eff}}{r}\left(\frac{1}{r}\frac{\partial w}{\partial \theta} + \frac{v}{r}\right) + \rho\frac{w^2}{r} + S^{v}_{spray} - \frac{\partial p}{\partial r}$
w (tangential velocity)	$\frac{\partial}{\partial x}\left(\frac{\mu_{eff}}{r}\frac{\partial u}{\partial \theta}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left[\mu_{eff}\, r\left(\frac{1}{r}\frac{\partial v}{\partial \theta} - \frac{w}{r}\right)\right] + \frac{1}{r}\frac{\partial}{\partial \theta}\left[\frac{\mu_{eff}}{r}\left(\frac{\partial w}{\partial \theta} + 2v\right)\right] - \frac{\rho v w}{r} + \frac{\mu_{eff}}{r}\left(\frac{\partial w}{\partial r} + \frac{\partial v}{r\partial \theta} - \frac{w}{r}\right) + S^{w}_{spray} - \frac{1}{r}\frac{\partial p}{\partial \theta}$
k (Turbulent kinetic energy)	$G_k - \rho\varepsilon$
ε (Dissipation rate)	$(C_1 G_k - C_2 \rho\varepsilon)\frac{\varepsilon}{k}$

TABLE E-1 (Contd)

Dependent Variable	Source Term
ϕ (Mixture fraction)	$\dot{m}_{evap}$
m_{fu} (Unburnt fuel mass fraction)	As per four-step mechanism, (Chapter VI) and modified by the eddy-break-up model as in Ref. 1, Page 23. $\dot{m}_{evap}$ added on to m_{fu} source.
m_{CH} (Intermedaite hydrocarbon mass fraction)	
m_{CO} (CO mass fraction)	
m_{H_2} (H_2 mass fraction)	
Soot nuclei and particle concentrations	As given in Chapter III, equations (28) and (29).
$\tilde{h}$ (Stagnation euthalpy)	$2a\,[(R^x - E) + (R^r - E) + (R^z - E)] + \dot{m}_{evap} H_{fuel}$

In the above table, the symbols have the meanings:

x, r, θ = axial, radial, tangential directions;

μ_{eff} = effective viscosity;

p = pressure;

ρ = density;

$$G_k = \mu_{eff} \left[2 \left\{ \left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial v}{\partial r}\right)^2 + \left(\frac{\partial w}{r\partial\theta} + \frac{v}{r}\right)^2 \right\} + \left(\frac{\partial w}{\partial x} + \frac{\partial u}{r\partial\theta}\right)^2 + \left(\frac{\partial u}{\partial r} + \frac{\partial v}{\partial x}\right)^2 + \left(\frac{\partial w}{\partial r} + \frac{\partial v}{r\partial\theta}\right) - \frac{w}{r}\right)^2 \right];$$

C_1, C_2 = Turbulence model constants;

S^u_{spray}, S^v_{spray}, S^w_{spray} = Momentum transfer from spray to the gas phase u, v, and w - momentum equations;

$\dot{m}_{evap}$ = rate of spray evaporation per unit volume;

a = Absorption coefficient defined as radiation absorbed per unit length;

E = Blackbody emissive power;

R^x, R^r, R^z = Composite radiation fluxes (See equations 37, 38, and 39);

H_{fuel} = Heat of formation of fuel.

APPENDIX F

INPUT DATA FOR JT8D-17 COMBUSTOR TEST CASE

APPENDIX F

INPUT DATA FOR JT8D-17 COMBUSTOR TEST CASE

In this Appendix, a listing of the input data used for the JT8D-17 Combustor computations is provided. The data shown is for the takeoff case using the four-step hydrocarbon oxidation mechanism. The specificaiton of the X, r, and θ grids is contained in lines 630-670. Other inputs may be easily interpreted with reference to the input description provided in Appendix B.

U-VELOCITY 10
V-VELOCITY 20
W-VELOCITY 30
PRESSURE 40
TURBULENT KINETIC ENERGY 50
TURBULENCE LENGTH SCALE 60
PHI (TOTAL FUEL) 70
FUEL MASS FRACTION 80
TEMPERATURE 90
SPECIFIC ENTHALPY 100
AVG. MAG. 110
PX 120
PY 130
PZ 140
CO 150
H2O 160
O2 170
CO2 160
N2 190
RHO 200
EFF. VISCOSITY 210
EVAPORATION RATE 220
NUCLEI CONCENTRATION 230
SOOT CONCENTRATION - SIZE 1 240
SOOT CONCENTRATION - SIZE 2 250
H 260
N 270
NO 280
NO2 290
O 300
OH 310
CXHY-2 320
H2 330
JTBD-COARSE GRID-TAKEOFF-JETA-4 STEP 340

10	10	05	02	02	02	02	03	350
01	02	00	00	00				360
01	01	01	01	01	01	01	01	370
01	01	01	01					380
								390
								400
01	01	01	03	01	01	01	01	410
01	01	01	01	01	01	01	01	420
01	01	01	01	01	01	01	01	430
01	01	01	01	01	01	01	01	440
01	01	01	00	00	00	01	01	450
01	00	00	00	00	00	01	00	460
00	00	00	00	00	00	00	00	470
	00	01	01	01	00	00	01	480
01								490
0.2	0.2	0.2	1.0	0.5	0.5	0.5	0.5	500
0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	510
0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	520
0.5	0.5	0.5	0.5	0.5	1.0	1.0	1.0	530
0.2	0.3	0.3						540
1.0	1.0	1.0	1.0	0.7	0.7	0.7	0.7	550
0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	560
0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	570
0.7	0.7	0.7	0.7	0.7	1.0	1.0	1.0	580
1.0	1.0	1.0	1.0	0.9	0.9	0.9	0.9	590
0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.9	600
0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.9	610
0.9	0.9	0.9	0.9	0.9	1.0	1.0	1.0	620
0.0	0.029	0.07	0.12	0.17	0.22	0.27	0.32	630
0.37	0.161							640

```
0.0       0.005     0.015     0.025     0.035     0.045     0.057     0.07
0.001     0.0064
0.0       0.1496    0.4488    0.7480    0.9376
02        15        09        10
1.7650E+06 1.0      0.1       0.01      0.003     0.02
10.       19.00     -49317.   .001
2.0893E+22 26000.   3.0       5.0117E+19 25000.   3.0
3.9811E+17 20000.   3.0       3.3113E+18 20500.   3.0
0.5       3.07      0.4       0.3       1.18      -0.37
1.0       0.25      0.5       0.85      1.42      -0.50
1.45      1.92      0.09      1.7100E-05 0.00001  713.6     713.6     713.6
075       100       04        04        00        02
46.418    0.3       1.16      0.081     0.0       713.6
01        02        300.0
.0001     .0001     0.4488    1.570795  -1.570795 0.0       5.83438   0.4498
5.00      0.01916   40.0      60.00     0.0
03        07
10        10
03        03
-80.0     -80.0
55.       55.
0.0001    0.0001
0.2620    0.7119
713.6     713.6
01        30        02
0.05      1.1000E+31 90000.   1.0000E+038.0000E-16 100.0    1.0000E-15 2000.0
1.5620E+13 16000.0  -1.94     1.81      -0.5      4.5000E+070.1       400.0
0.025     1.0
90.0      10.0
30        0.001
01        99        02        0.0005    500.0
ELEMENTS
C         12.01115  4.000000
H          1.007970 1.000000
N         14.006700 0.0
O         15.999400-2.000000

THERMO
C10H19              J 3/61C 10.H 19.00 0.00 0.G   300.000  5000.000
 0.26845936E+02 0.46470050E-01-0.22967813E-04 0.48494616E-08-0.37080219E-12
-0.24819829E+05 0.10707143E+02 0.57799475E+01 0.50561468E-01 0.51144255E-04
-0.94968140E-07 0.39603875E-10-0.24819829E+05 0.86690068E+00
O2                  J 9/65O 2.0  0.0  0.0  0.G    300.000  5000.000
 0.36219521E 01 0.73618256E-03-0.19652219E-06 0.36201556E-10-0.28945023E-14
-0.12019422E 04 0.36150942E 01 0.36255980E 01-0.18782183E-02 0.70554543E-05
-0.67635371E-08 0.21555977E-11-0.10475225E 04 0.43052769E 01
N2                  J 9/65N  2.0  0.0  0.0  0.G    300.000  5000.000
 0.28963194E 01 0.15154863E-02-0.57235275E-06 0.99807385E-10-0.65223536E-14
-0.90586182E 03 0.61615143E 01 0.36748257E 01-0.12081496E-02 0.23240100E-05
-0.63217520E-09-0.22577253E-12-0.10611587E 04 0.23580418E 01
CO                  J 9/65C  1.0  1.00 0.00 0.G   300.000  5000.000
 0.29840699E 01 0.14891387E-02-0.57899678E-06 0.10364576E-09-0.69353499E-14
-0.14245227E 05 0.63479147E 01 0.37100916E 01-0.16190964E-02 0.36923584E-05
-0.20319673E-08 0.23953344E-12-0.14355309E 05 0.29555340E 01
C2H4                J 3/61C 2.0H 4.000 0.00 0.G   300.000  5000.000
 2.23312189E+00 1.32141704E-02-5.11224078E-06 8.83920914E-10-5.63643039E-14
 5.10533922E+03 9.38961110E+00 2.41824020E+00 1.22921229E-02-4.24080270E-06
 2.13889578E-09-1.44584497E-12 5.05491829E+03 9.02623340E+00
H2                  J 3/61H  2.0  0.0  0.0  0.G   300.000  5000.000
 0.31001883E 01 0.51119459E-03 0.52644204E-07-0.34909964E-10 0.36945341E-14
-0.87730613E 03-0.19629421E 01 0.30574446E 01 0.26765198E-02-0.58099145E-05
 0.55210343E-08-0.18122726E-11-0.98890430E 03-0.22997046E 01
H2O                 J 3/61H  2.0  1.00 0.00 0.G   300.000  5000.000
 0.27167610E 01 0.29451370E-02-0.80224368E-06 0.10226681E-09-0.48472134E-14
```

```
-0.25905320E 05 0.66305666E 01 0.40701275E 01-0.11684599E-02 0.41521160E-05
-0.29637434E-08 0.30762101E-12-0.30279719E 05-0.32270040E 00
CO2                 J 9/65C  1.0  2.00 0.00 0.0   300.000  5000.000
 0.44608040E 01 0.30981717E-02-0.12392566E-05 0.22741325E-09-0.15525954E-13
-0.48961430E 05-0.98635978E 00 0.24007784E 01 0.87350958E-02-0.66070861E-05
 0.20021860E-08 0.63274039E-15-0.48377520E 05 0.96951457E 01
H                   J 9/65H  1.00 0.00 0.00 0.0   300.000  5000.000
 0.25000000E 01 0.0             0.0             0.0             0.0
 0.25471625E 05-0.46011759E 00 0.25000000E 01 0.0             0.0
 0.0            0.0             0.25471625E 05-0.46011759E 00
N                   J 3/61N  1.00 0.00 0.00 0.0   300.000  5000.000
 0.24502678E 01 0.10661450E-03-0.74653315E-07 0.18795520E-10-0.10259837E-14
 0.56116035E 05 0.44487572E 01 0.25030699E 01-0.21800181E-04 0.54205284E-07
-0.56475602E-10 0.20999040E-13 0.56098890E 05 0.41675749E 01
NO                  J 6/63N  1.0  1.00 0.00 0.0   300.000  5000.000
 0.31889992E 01 0.13382278E-02-0.52899318E-06 0.95919316E-10-0.64847920E-14
 0.98283242E 04 0.67458115E 01 0.40459509E 01-0.34181783E-02 0.79819176E-05
-0.61113925E-08 0.15919072E-11 0.97453867E 04 0.29974976E 01
NO2                 J 9/64N  1.0  2.00 0.00 0.0   300.000  5000.000
 0.46240759E 01 0.25260330E-02-0.10609483E-05 0.19877239E-09-0.13799390E-13
 0.22899760E 04 0.13324137E 01 0.34589224E 01 0.20647063E-02 0.66866001E-05
-0.95556665E-08 0.36199873E-11 0.28152261E 04 0.83116980E 01
O                   J 6/62O  1.00 0.00 0.00 0.0   300.000  5000.000
 0.25420596E 01-0.27550619E-04-0.31028029E-08 0.45510670E-11-0.43680434E-15
 0.29230800E 05 0.49203072E 01 0.29466289E 01-0.16381664E-02 0.24210303E-05
-0.16028432E-08 0.38906964E-12 0.29147644E 05 0.29639931E 01
OH                  J 3/66O  1.0  1.00 0.00 0.0   300.000  5000.000
 0.29106417E 01 0.95931627E-03-0.19441700E-06 0.13756646E-10 0.14224542E-15
 0.39353811E 04 0.54423420E 01 0.38375931E 01-0.10773059E-02 0.96830354E-06
 0.18713971E-09-0.22571389E-12 0.36412829E 04 0.49370009E 00

MECHANISM
C10H19                               C2H4      H2                                                G108
C2H4      O2                         CO        H2                                                G108
CO        O2                         CO2                                                         G108
H2        O2                         H2O                                                         G108
H         H          M               H2                   M        12.3     -1.0  0.0      0.0
O         O          M               O2                   M        11.0     -1.0  0.0      0.0
H         OH         M               H2O                  M        13.85    -1.0  0.0      0.0
H         O2                         OH        O                   11.35     0.0  8400.    0.0
O         H2                         OH        H                   10.24     0.0  4720.    0.0
H         H2O                        OH        H2                  10.92     0.0  10050.   0.0
O         H2O                        OH        OH                  10.70     0.0  9000.    0.0
N2        O                          NO        N                   9.0       0.0  25000.   0.0
N         O2                         NO        O                   9.800     1.0  2000.    0.0
N         OH                         NO        H                   9.000     0.0  0.0      0.0
N2        O2                         N         NO2                 11.931   -1.0  50000.   0.0
NO        NO                         N         NO2                 7.00      0.0  0.0      0.0
NO        O2                         NO2       O                   9.0       0.0  22900.   0.0
H         NO2                        NO        OH                  10.477    0.0  0.0      0.0
```

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APPENDIX G

DIMENSIONS OF VARIABLE ARRAYS

APPENDIX G

DIMENSIONS OF VARIABLE ARRAYS

The program listing shown in Appendix D is for a 10 x 10 x 5 (axial x radial x tangential) grid. In order to change the number of nodes to any NX, NY, NZ, the dimensions of various variable arrays have to be changed as indicated on the following page. Some of the variables are dimensioned as (NX, NY, NZ) in some subroutines and as (NXYZ) in others. Both forms are indicated below. In addition, in BLOCK DATA, NI, NJ, and NK have to be set to NX, NY, and NZ, respectively.

```
NXYZ = NX*NY*NZ
NXY  = NX*NY
```

Variable	Dimensions
F	(NXYZ, 7) or (7* NXYZ)
DU, DV, DW, ANUC, SOOT1, SOOT2, FCH, FH2, RHO, VISC, ABSR, SCTR, DRHODP, U, V, W, PP, P, TEMP, GAM	(NX, NY, NZ) or (NXYZ)
FS	(NXYZ, 14)
GENR, SUFU, SPFU	(NXYZ)
SU, SP, AXP, AXM, AYP, AYM, AZP, AZM, CZ, CZU, CZP, DIVG	(NX, NY) or (NXY)
AXMK, AXPK, AYMK, AYPK, AZMK, AZPK, SUK, SPK, EVAP, EVAPU, EVAPV, EVAPW, EDK, EDK 2	(NX-2)*(NY-2)*(NZ-2)
EVSU	(NX-2)*(NY-2)
CY, CYU, CYP, X, XS, XSU, XDIF, FXP, FXM, FLO, TEMTM, H, FUEL, FUOX, UIN, TIN, FUELS	GE.(NX)
R, RM, RMV, YSR, YSVR, Y, YS, YSV YDIF, FYP, FYM, JM	GE·(NY)
Z, ZS, ZSW, ZDIF, FZP, FZM, KM	GE·(NZ)
IWLI, IWLO	GE·(NY, 5)
JWLO, JWLI	GE·(NX, 5)
JKIN	GE.(NY, NZ)
IKIN	GE·(NX, NZ)